Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 02	LMEDLINE coverage updated
NEWS 3	JUL 02	SCISEARCH enhanced with complete author names
NEWS 4	JUL 02	CHEMCATS accession numbers revised
NEWS 5	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 6	JUL 16	CAplus enhanced with French and German abstracts
NEWS 7	JUL 18	CA/CAplus patent coverage enhanced
NEWS 8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9	JUL 30	USGENE now available on STN
NEWS 10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 11	AUG 06	BEILSTEIN updated with new compounds
NEWS 12	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 13	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 14	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 15	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 16	AUG 27	USPATOLD now available on STN
NEWS 17	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 18	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 19	SEP 13	FORIS renamed to SOFIS
NEWS 20	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 21	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 22	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 23	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:23:46 ON 27 SEP 2007

=> FILE REG
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:23:58 ON 27 SEP 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 SEP 2007 HIGHEST RN 948239-70-1
DICTIONARY FILE UPDATES: 26 SEP 2007 HIGHEST RN 948239-70-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

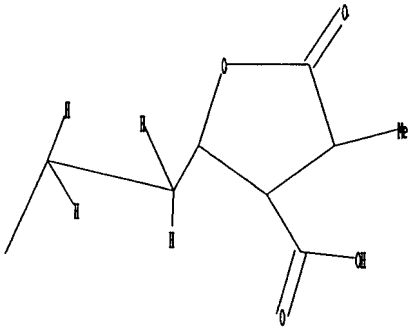
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

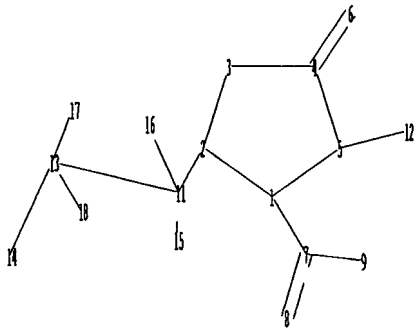
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519804b.str





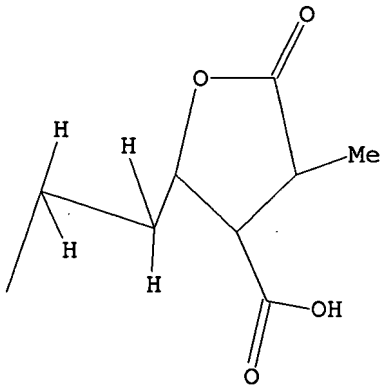
chain nodes :
6 7 8 9 13 14 15 16 17 18
ring nodes :
1 2 3 4 5
ring/chain nodes :
11 12
chain bonds :
1-7 2-11 4-6 5-12 7-8 7-9 11-13 11-15 11-16 13-14 13-17 13-18
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
4-6
exact bonds :
1-2 1-5 1-7 2-3 2-11 3-4 4-5 5-12 11-13 11-15 11-16 13-14 13-17 13-18

normalized bonds :
7-8 7-9
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 09:24:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 24 TO ITERATE

100.0% PROCESSED 24 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 187 TO 773
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 09:24:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 545 TO ITERATE

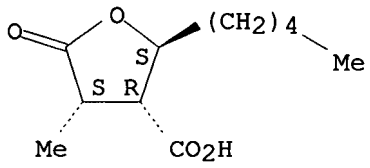
100.0% PROCESSED 545 ITERATIONS 53 ANSWERS
SEARCH TIME: 00.00.01

L3 53 SEA SSS FUL L1

=> d scan

L3 53 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3R,4S)-
MF C11 H18 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 09:24:48 ON 27 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 27 Sep 2007 VOL 147 ISS 14
FILE LAST UPDATED: 26 Sep 2007 (20070926/ED)

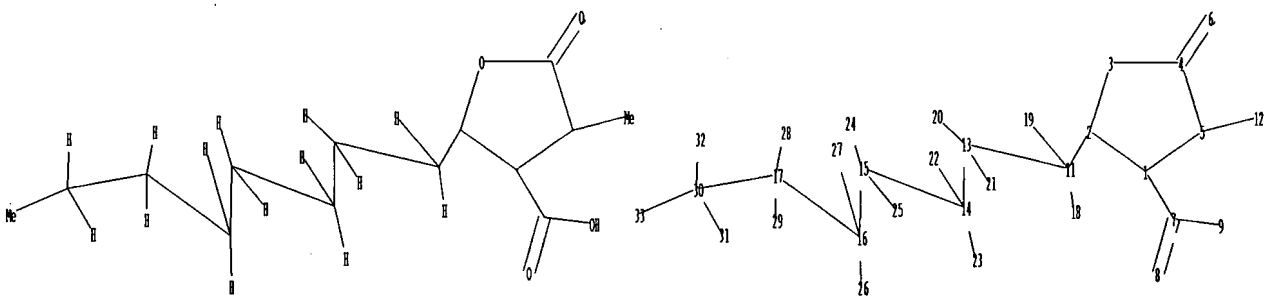
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3 full
L4 73 L3

=> s l4 and py<2002
  21900255 PY<2002
L5 53 L4 AND PY<2002

=>
Uploading C:\Program Files\Stnexp\Queries\10519804.str



chain nodes :
6 7 8 9 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33
ring nodes :
1 2 3 4 5
ring/chain nodes :
11 12
chain bonds :
1-7 2-11 4-6 5-12 7-8 7-9 11-13 11-18 11-19 13-14 13-20 13-21 14-15 14-22 14-23 15-16 15-24 15-25 16-17 16-26 16-27 17-28 17-29 17-30 30-31 30-32 30-33
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
4-6
exact bonds :
1-2 1-5 1-7 2-3 2-11 3-4 4-5 5-12 11-13 11-18 11-19 13-14 13-20 13-21 14-15 14-22 14-23 15-16 15-24 15-25 16-17 16-26 16-27 17-28 17-29 17-30 30-31 30-32 30-33
normalized bonds :
7-8 7-9
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS

L6 STRUCTURE UPLOADED

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.30	177.61

FILE 'REGISTRY' ENTERED AT 09:29:07 ON 27 SEP 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 SEP 2007 HIGHEST RN 948239-70-1
DICTIONARY FILE UPDATES: 26 SEP 2007 HIGHEST RN 948239-70-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

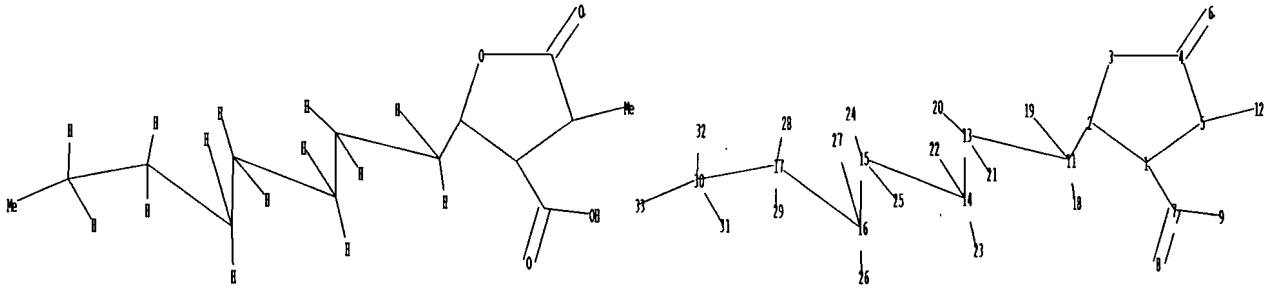
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519804.str



chain nodes :
6 7 8 9 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33
ring nodes :
1 2 3 4 5
ring/chain nodes :
11 12
chain bonds :
1-7 2-11 4-6 5-12 7-8 7-9 11-13 11-18 11-19 13-14 13-20 13-21 14-15 14-22 14-23 15-16 15-24 15-25 16-17 16-26 16-27 17-28 17-29 17-30 30-31 30-32 30-33
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
4-6
exact bonds :
1-2 1-5 1-7 2-3 2-11 3-4 4-5 5-12 11-13 11-18 11-19 13-14 13-20 13-21 14-15 14-22 14-23 15-16 15-24 15-25 16-17 16-26 16-27 17-28 17-29 17-30 30-31 30-32 30-33
normalized bonds :
7-8 7-9
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS

L7 STRUCTURE UPLOADED

=> s l7 full
FULL SEARCH INITIATED 09:29:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 301 TO ITERATE

100.0% PROCESSED 301 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

L8 5 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 349.71

FILE 'CAPLUS' ENTERED AT 09:29:29 ON 27 SEP 2007

FILE COVERS 1907 - 27 Sep 2007 VOL 147 ISS 14
FILE LAST UPDATED: 26 Sep 2007 (20070926/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

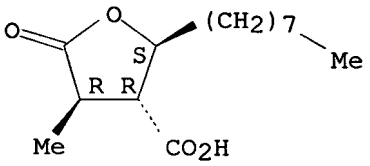
=> s l8 full
L9 4 L8

=> d ibib abs hitstr tot

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:708473 CAPLUS
DOCUMENT NUMBER: 143:326143
TITLE: New α-methylene-γ-butyrolactones with antimycobacterial properties
AUTHOR(S): Hughes, Minerva A.; McFadden, Jill M.; Townsend, Craig A.
CORPORATE SOURCE: Department of Chemistry, The Johns Hopkins University, Baltimore, MD, 21218, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(17), 3857-3859
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:326143
AB The synthesis and antimycobacterial activity of a series of α-methylene-γ-butyrolactones based on the natural product protolichesterinic acid are described. The products bearing an allylamide group at the C-4 position showed improved activity with MICs in the range of 6.25-12.5 μg/mL.
IT 647830-52-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of α-methylene-γ-butyrolactone derivs. and study of their antimycobacterial activity)
RN 647830-52-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



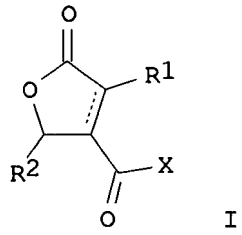
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:60242 CAPLUS
DOCUMENT NUMBER: 140:111267
TITLE: Preparation of γ-butyrolactone-4-carboxylate derivatives as inhibitors of fatty acid synthase
INVENTOR(S): Kuhadja, Francis P.; Medghalchi, Susan M.; Thupari, Jagan N.; Townsend, Craig A.; McFadden, Jill M.
PATENT ASSIGNEE(S): Fasgen, Llc., USA; The Johns Hopkins University
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

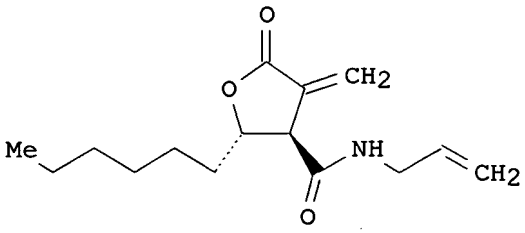
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004006835	A2	20040122	WO 2003-US20960	20030701
WO 2004006835	A3	20040722		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2491183	A1	20040122	CA 2003-2491183	20030701
AU 2003248810	A1	20040202	AU 2003-248810	20030701
EP 1534263	A2	20050601	EP 2003-764343	20030701
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005533107	T	20051104	JP 2004-521521	20030701

CN 1705478	A	20051207	CN 2003-818369		20030701
IN 2004KN02001	A	20070309	IN 2004-KN2001		20041229
US 2006241177	A1	20061026	US 2006-519804		20060519
PRIORITY APPLN. INFO.:			US 2002-392809P	P	20020701
			WO 2003-US20960	W	20030701

OTHER SOURCE(S): MARPAT 140:111267
GI



I



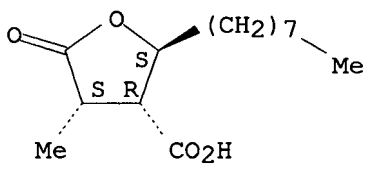
II

AB The title compds. I [R1 = H, (cyclo)alkyl, alkenyl, (alkyl)aryl, etc.; R2 = (cyclo)alkyl, alkenyl, (alkyl)aryl, etc.; X = OR3 or NHR3, where R3 = H, (cyclo)alkyl, alkenyl, (alkyl)aryl, etc.] were prepared as inhibitors of fatty acid synthase and neuropeptide-Y for weight loss, anti-microbial and anti-cancer applications. Thus, reaction of (±)-α-methylene-γ-butyrolactone-5-hexyl-4-carboxylic acid with allylamine yielded compound II. The latter inhibits human fatty acid synthase with IC50 = 81 μg/mL.

IT 647830-51-1P 647830-52-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of γ-butyrolactone carboxylate derivs. as inhibitors of fatty acid synthase)

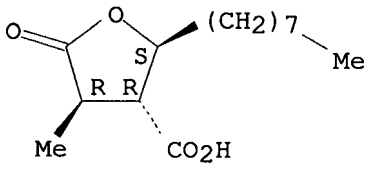
RN 647830-51-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2R,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



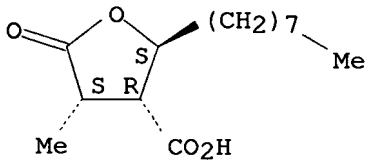
RN 647830-52-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



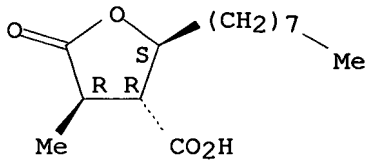
IT 647830-61-3P 647830-62-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of γ-butyrolactone carboxylate derivs. as inhibitors of fatty acid synthase)
RN 647830-61-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2S,3R,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 647830-62-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:885658 CAPLUS
DOCUMENT NUMBER: 140:156943
TITLE: Fatty Acid Synthase Inhibition Triggers Apoptosis during S Phase in Human Cancer Cells
AUTHOR(S): Zhou, Weibo; Simpson, P. Jeanette; McFadden, Jill M.; Townsend, Craig A.; Medghalchi, Susan M.; Vadlamudi, Aravinda; Pinn, Michael L.; Ronnett, Gabriele V.; Kuhajda, Francis P.
CORPORATE SOURCE: Department of Pathology, The Johns Hopkins University School of Medicine, Baltimore, MD, 21205, USA
SOURCE: Cancer Research (2003), 63(21), 7330-7337
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
AB C75, an inhibitor of fatty acid synthase (FAS), induces apoptosis in

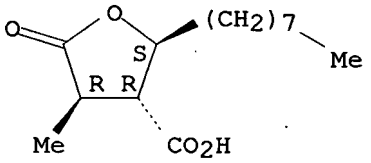
cultured human cancer cells. Its proposed mechanism of action linked high levels of malonyl-CoA after FAS inhibition to potential downstream effects including inhibition of carnitine palmitoyltransferase-1 (CPT-1) with resultant inhibition of fatty acid oxidation Recent data has shown that C75 directly stimulates CPT-1 increasing fatty acid oxidation in MCF-7 human breast cancer cells despite inhibitory concns. of malonyl-CoA. In light of these findings, we have studied fatty acid metabolism in MCF7 human breast cancer cells to elucidate the mechanism of action of C75. We now report that: (a) in the setting of increased fatty acid oxidation, C75 inhibits fatty acid synthesis; (b) C273, a reduced form of C75, is unable to inhibit fatty acid synthesis and is nontoxic to MCF7 cells; (c) C75 and 5-(tetradecyloxy)-2-furoic acid (TOFA), an inhibitor of acetyl-CoA carboxylase, both cause a significant reduction of fatty acid incorporation into phosphatidylcholine, the major membrane phospholipid, within 2 h; (d) pulse chase studies with [14C]acetate labeling of membrane lipids show that both C75 and TOFA accelerate the decay of 14C-labeled lipid from membranes within 2 h; (e) C75 also promotes a 2-3-fold increase in oxidation of membrane lipids within 2 h; and (f) because interference with phospholipid synthesis during S phase is known to trigger apoptosis in cycling cells, we performed double-labeled terminal deoxynucleotidyltransferase-mediated nick end labeling and BrdUrd anal. with both TOFA and C75. C75 triggered apoptosis during S phase, whereas TOFA did not. Moreover, application of TOFA 2 h before C75 blocked the C75 induced apoptosis, whereas etomoxir did not. Taken together these data indicate that FAS inhibition and its downstream inhibition of phospholipid production is a necessary part of the mechanism of action of C75. CPT-1 stimulation does not likely play a role in the cytotoxic response. The continued ability of TOFA to rescue cancer cells from C75 cytotoxicity implies a proapoptotic role for malonyl-CoA independent of CPT-1 that selectively targets cancer cells as they progress into S phase.

IT 647830-62-4, C 273
RL: PAC (Pharmacological activity); BIOL (Biological study)
(fatty acid synthase inhibition triggers apoptosis during S phase in human cancer cells)

RN 647830-62-4 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1939:14245 CAPLUS

DOCUMENT NUMBER: 33:14245

ORIGINAL REFERENCE NO.: 33:2125a-f

TITLE: Constitution of nephromopsinic acid. II

AUTHOR(S): Asano, Mitizo; Azumi, Tiaki

SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1939), 72B, 35-9
CODEN: BDCBAD; ISSN: 0365-9488

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

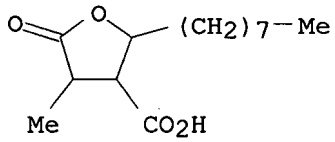
GI For diagram(s), see printed CA Issue.

AB cf. C. A. 29, 5072.6. When nephromopsinic acid, C19H34O4 (I), which is probably a diastereomer of dihydroprotolichesterinic acid, RC4H.C3H(CO2H).C2HMe.C1O.O (II, R = C13H27), is heated with 2 equivs. of alc. KOH so that the lactone ring is opened and is then treated with AgNO3 it gives a gray-black Ag salt which with MeI yields the Me ester, m. 59-60°, of I, identical with that obtained with CH2N2. On the other hand, saponification of this ester with alc. KOH does not regenerate the original I but l-II, m. 103-5°. As II is formed by hydrogenation of protolichesterinic acid, it must be assumed that the 2-C atom of II is racemized. It follows that alkaline saponification of I opens the lactone ring, to be sure, but does not racemize the 2-C atom; when, however, its ester is saponified, the 2-C atom is first enolized and on acidification II is formed. α-Methyl-γ-alkylparaconic acids (II) were synthesized according to the scheme RCOCH2CO2Et + MeCHBrCO2Et (III) → RCOCH(CO2Et)CHMeCO2Et (+ Na-Hg) → II. From 6 g. Et pelargonoylacetate (IV), b16 149-51°, b2 115°, with III and Na in alc. at 120° was obtained 8 g. di-Et α-methyl-α'-pelargonoylsuccinate (V), b3 158-62°, which gives a faint brown color with alc. FeCl3. The residue from the distillation of IV solidified on long standing and yielded from AcOH tablets of 6-octyl-3-pelargonoylpyronone, m. 70-1°, insol. in alkali and giving no color with FeCl3. V (20 g.) in alc. and water treated in the course of 3 days with Na-Hg with occasional addns. of AcOH to tone down the alkalinity gave about 8 g. acid products which on esterification yielded 1 g. α-methyl-γ-octylparaconic acid (VI), m. 112-14°, and a mixture of esters separated into 4 g. b2 130-60° (VII) and 2 g. b2 164-70° (VIII). Saponification of VII yielded α-methyl-γ-ketolauric acid, m. 62-3° (semicarbazone, m. 125-6.5°), and VIII gave VI. Heated with Na in alc. at 90-100° and then saponified with 5% KOH VIII yielded α-methyl-α'-nonylidenesuccinic acid, m. 132-4°, which immediately decolorized KMnO4. Et myristoylacetate (IX), b3 165-70°; in its distillation there remained a considerable residue of 6-tridecyl-3-myristoylpyronone, m. 85.5-7°, which with HI (d. 1.7) at 160-70° yielded ditridecylpyronone, m. 65-6°. α'-Myristoyl homolog of V (34 g. from 28 g. IX), brownish oil, gave with Na-Hg lichesterylic acid, m. 80-3°, and a little (0.1 g.) of the γ-tridecyl homolog of VI, m. 143-6°.

IT 854909-07-2P, Paraconic acid, 4-methyl-2-octyl-
RL: PREP (Preparation)
(preparation of)

RN 854909-07-2 CAPLUS

CN Paraconic acid, 4-methyl-2-octyl- (4CI) (CA INDEX NAME)



=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	21.55	371.26

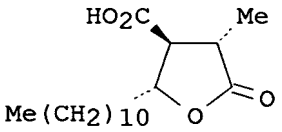
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.12	-3.12

FILE 'STNGUIDE' ENTERED AT 09:29:55 ON 27 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

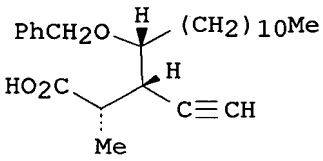
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Sep 24, 2007 (20070924/UP).

=> d ibib abs hitstr l5 1-20
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L5 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:34084 CAPLUS
DOCUMENT NUMBER: 136:294668
TITLE: Enantioselective syntheses of (+)- and (-)-nephrosteranic acid employing the Nicholas-Schreiber reaction
AUTHOR(S): Jacobi, Peter A.; Herradura, Prudencio
CORPORATE SOURCE: Dep. Chem., Dartmouth College, Hanover, NH, 03755, USA
SOURCE: Canadian Journal of Chemistry (2001), 79(11), 1727-1735
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:294668
GI



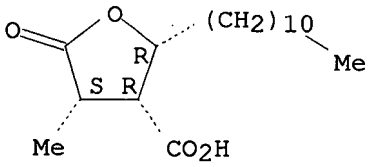
I



II

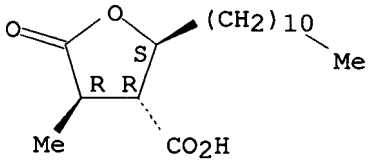
AB (+)- And (-)-Nephrosteranic acid (I) have been prepared in an enantioselective fashion from alkyne acid II (or ent-II) by a three step sequence involving debenzylation-lactonization, oxidative cleavage, and selective epimerization at C4. Acids II and ent-II were obtained as single enantiomers employing a Nicholas-Schreiber reaction.
IT 405552-35-4P, (+)-4-epi-Nephrosteranic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective syntheses of (+)- and (-)-nephrosteranic acid via the Nicholas-Schreiber reaction)
RN 405552-35-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3R,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



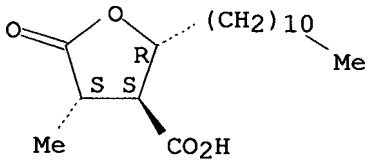
IT 480-71-7P, (-)-Nephrosteranic acid 70579-56-5P, (+)-Nephrosteranic acid 407635-98-7P, (-)-4-epi-Nephrosteranic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective syntheses of (+)- and (-)-nephrosteranic acid via the Nicholas-Schreiber reaction)
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



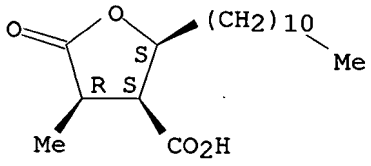
RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 407635-98-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

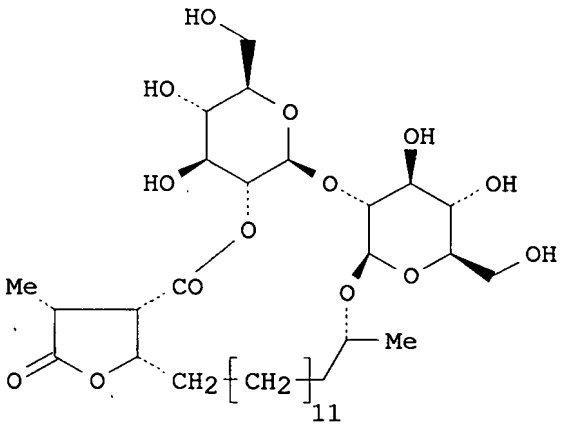
L5 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:883604 CAPLUS
DOCUMENT NUMBER: 136:229116

TITLE: Macrolactone glycosides of three lichen acids from Acarospora gobiensis, a lichen of Central Asia

AUTHOR(S): Rezanka, Tomas; Guschina, Irina A.
CORPORATE SOURCE: Institute of Microbiology, Prague, 14220, Czech Rep.

SOURCE: Phytochemistry (2001), 58(8), 1281-1287
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

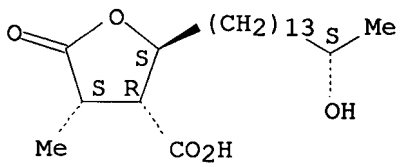
AB The compds. isolated from the extract of Central Asian lichen (Acarospora gobiensis H. Magn.) comprised three new glycosides having 18-hydroxy-dihydroalloprotolichesterinic, 18-hydroxy-neodihydroprotolichesterinic and 18-hydroxy-dihydroprotolichesterinic acids as aglycons and a di- or trisaccharide moiety linked at C-18 and at the carboxylic group. These compds., called gobienines A-C (e.g I, gobienine A), were found to be di- or trisaccharides forming a macrolactone with the aglycon. The structures were elucidated by using extensive spectroscopic anal. (1D and 2D NMR, MS, IR and ORD) and chemical and enzymic methods.

IT 379224-47-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (18S-hydroxydihydroprotolichesterinic acid; gobienine B hydrolysis product)

RN 379224-47-2 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4S)- (9CI) (CA INDEX NAME)

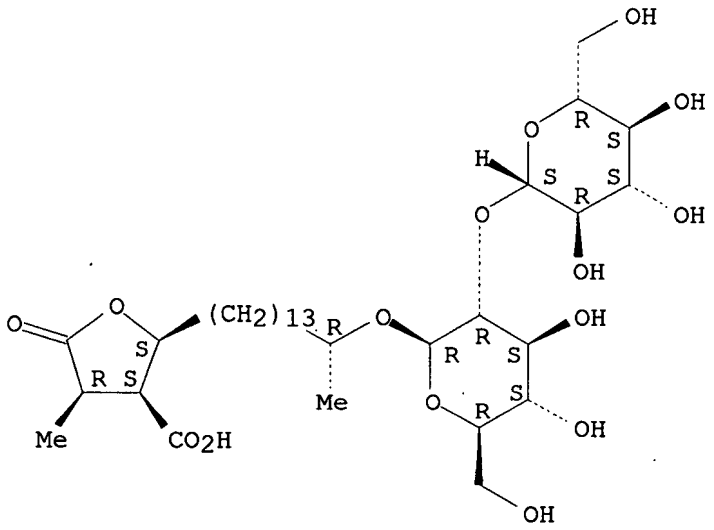
Absolute stereochemistry. Rotation (+).



IT 403618-80-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (gobienine A esterase treatment product)

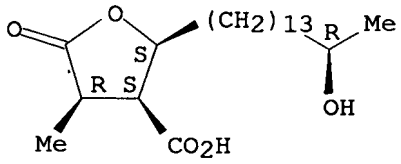
RN 403618-80-4 CAPLUS
CN 3-Furancarboxylic acid, 2-[(14R)-14-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]pentadecyl]tetrahydro-4-methyl-5-oxo-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



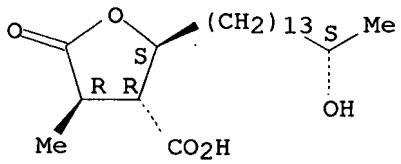
IT 379224-46-1P, 18R-Hydroxydihydroalloprotolichesterinic acid
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(gobienine A hydrolysis product)
RN 379224-46-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



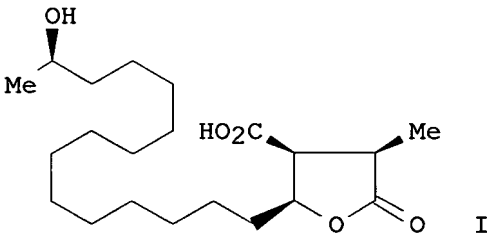
IT 379224-48-3P, 18S-Hydroxyneodihydroprotolichesterinic acid
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(gobienine B hydrolysis product)
RN 379224-48-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

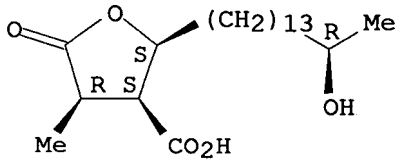
L5 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:667445 CAPLUS
DOCUMENT NUMBER: 136:17754
TITLE: Glycoside esters from lichens of central Asia
AUTHOR(S): Rezanka, T.; Guschina, I. A.
CORPORATE SOURCE: Institute of Microbiology, Prague, 14220, Czech Rep.
SOURCE: Phytochemistry (2001), 58(3), 509-516
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

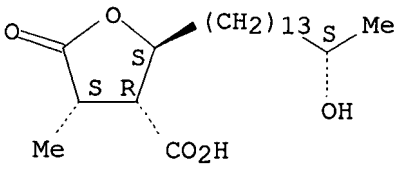
AB Ten compds. (e.g. I) isolated from the extract of the central Asian lichens comprised new glycosides and glycoside esters having 18R-hydroxy-dihydroalloprotolichesterinic, 18S-hydroxy-dihydroprotolichesterinic and 18S-hydroxy-neodihydroprotolichesterinic acids, as the aglycons and a saccharide moiety linked at C-18 and also at C-21 made by glucose, xylose or rhamnose. The structures were elucidated using extensive spectroscopic anal. (1D and 2D NMR, MS, IR, UV and ORD) and by biochem. methods.
IT 379224-46-1P, 18R-Hydroxydihydroalloprotolichesterinic acid
379224-47-2P, 18S-Hydroxydihydroprotolichesterinic acid
379224-48-3P, 18S-Hydroxyneodihydroprotolichesterinic acid
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(glycoside esters from lichens of central Asia)
RN 379224-46-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



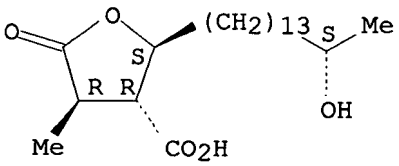
RN 379224-47-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 379224-48-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4R)- (9CI) (CA INDEX NAME)

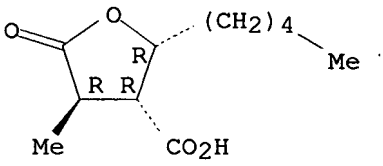
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:321140 CAPLUS
DOCUMENT NUMBER: 135:107173
TITLE: A concise synthesis of (±)-methylenolactocin and the formal synthesis of (±)-phaseolinic acid
AUTHOR(S): Loh, T.-P.; Lye, P.-L.
CORPORATE SOURCE: Department of Chemistry, The National University of Singapore, Singapore, 117543, Singapore
SOURCE: Tetrahedron Letters (2001), 42(20), 3511-3514
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:107173
AB (±)-Methylenolactocin was prepared in five steps involving an indium-mediated allylation reaction as the key step.
IT 203514-35-6P, (±)-Phaseolinic acid
RL: PNU (Preparation, unclassified); PREP (Preparation)
(synthesis of (±)-methylenolactocin and formal synthesis of (±)-phaseolinic acid via indium-mediated allylation)
RN 203514-35-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



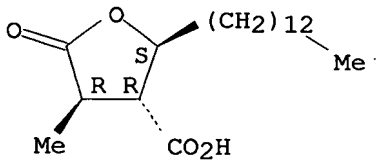
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:238464 CAPLUS
DOCUMENT NUMBER: 135:33403
TITLE: Enantioselective Synthesis of (-)-Roccellaric Acid
AUTHOR(S): Boehm, Claudius; Reiser, Oliver
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Regensburg, Regensburg, 93053, Germany
SOURCE: Organic Letters (2001), 3(9), 1315-1318
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:33403

AB A new strategy for the synthesis of anti-4,5-disubstituted γ-butyrolactones starting from inexpensive furan-2-carboxylic Me ester was developed. By applying this methodol., the enantioselective synthesis of (-)-roccellaric acid was accomplished using a copper(I)-catalyzed asym. cyclopropanation, a tin(IV)-catalyzed retroaldol/lactonization sequence of cyclopropanols, and a ruthenium-catalyzed intermol. metathesis reaction as key steps.

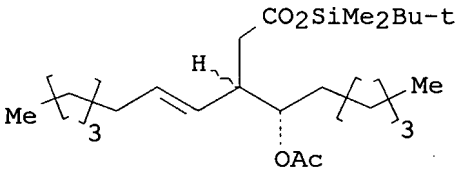
IT 148676-05-5P, (-)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of the γ-butyrolactone (-)-roccellaric acid)
RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:61277 CAPLUS
DOCUMENT NUMBER: 134:252178
TITLE: A concise synthesis of (-)-methylenolactocin and (-)-phaseolinic acid from (6S,9S)-tetradec-7-yne-6,9-diol
AUTHOR(S): Ariza, Xavier; Garcia, Jordi; Lopez, Marta; Montserrat, Laia
CORPORATE SOURCE: Departament de Quimica Organica, Div. III, Universitat de Barcelona, Barcelona, 08028, Spain
SOURCE: Synlett (2001), (1), 120-122
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:252178
GI



I

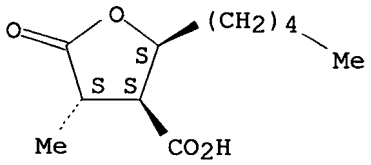
AB A novel, stereodivergent route to paraconic acids from C2-sym. trans- and cis-alk-2-ene-1,4-diols through Ireland-Claisen and/or Johnson ortho ester I (threo = β-H; erythro = α-H) rearrangements was accomplished. This strategy was applied to the synthesis of (-)-methylenolactocin and (-)-phaseolinic acid from the chiral title diol.

IT 109667-12-1P, (-)-Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (-)-methylenolactocin and (-)-phaseolinic acid from (6S,9S)-tetradec-7-yne-6,9-diol)

RN 109667-12-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:85990 CAPLUS

DOCUMENT NUMBER: 132:236929

TITLE: Asymmetric carbolithiation of 2-phenylselenofumarate derivatives: a short synthesis of (-)-roccellaric acid

AUTHOR(S): Bella, Marco; Margarita, Roberto; Orlando, Claudia; Orsini, Monica; Parlanti, Luca; Piancatelli, Giovanni

CORPORATE SOURCE: Dipartimento di Chimica, Universita "La Sapienza", Rome, 00185, Italy

SOURCE: Tetrahedron Letters (2000), 41(4), 561-565
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:236929

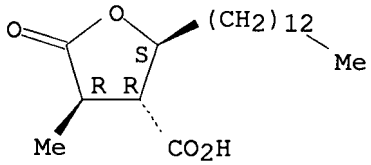
AB (-)-Roccellaric acid and variously substituted succinates are obtained through direct asym. carbolithiation of 2-phenylselenofumarate derivs., followed by reaction with suitable electrophiles.

IT 148676-05-5P, (-)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of (-)-roccellaric acid via asym. carbolithiation of 2-phenylselenofumarate derivs.)

RN 148676-05-5 CAPLUS

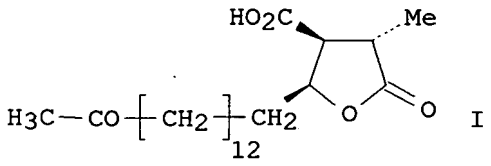
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:665856 CAPLUS
DOCUMENT NUMBER: 132:33194
TITLE: A Revised Structure for (-)-Dihydropertusaric Acid, a γ-Butyrolactone Acid from the Lichen Punctelia microsticta
AUTHOR(S): Maier, Marta S.; Gonzalez Marimon, Diego I.; Stortz, Carlos A.; Adler, Monica T.
CORPORATE SOURCE: Departamento de Quimica Organica and Departamento de Ciencias Biologicas, Facultad de Ciencias Exactas y Naturales, Buenos Aires, 1428, Argent.
SOURCE: Journal of Natural Products (1999), 62(11), 1565-1567
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



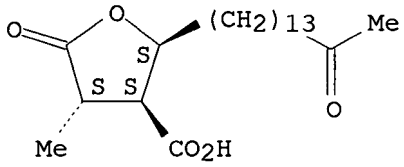
I

AB The γ-butyrolactone acid, (-)-dihydropertusaric acid (I), and two known compds., (-)-isomuronic acid and the tridepside gyrophoric acid, were isolated from the lichen Punctelia microsticta. The structure and stereochem. of I were determined on the basis of spectroscopic evidence and mol. modeling. Spectroscopic and phys. data of I were identical with those of a previously isolated compound from the lichen Pertusaria albescens which had been reported with a different relative configuration.

IT 101899-68-7P, (-)-Dihydropertusaric acid
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)
(isolation, mol. structure, conformation, and revised configuration for (-)-dihydropertusaric acid, a γ-butyrolactone acid from the lichen Punctelia microsticta)

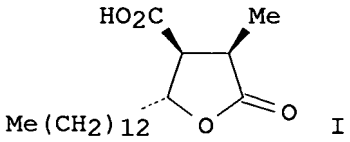
RN 101899-68-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2S,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:602818 CAPLUS
DOCUMENT NUMBER: 131:336854
TITLE: Total synthesis of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid by radical cyclization of an epoxide using a transition-metal radical source
AUTHOR(S): Mandal, Pijus Kumar; Roy, Subhas Chandra
CORPORATE SOURCE: Department of Organic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700032, India
SOURCE: Tetrahedron (1999), 55(37), 11395-11398
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:336854
GI

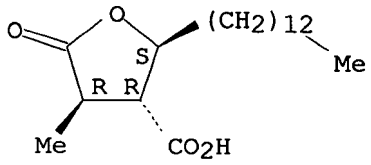


I

AB A short and efficient total synthesis of (±)-dihydroprotolichesterinic acid (I) and the formal synthesis of (±)-rocellaric acid were achieved by radical cyclization of an epoxide using a transition metal radical source.

IT 220379-59-9P, (±)-Rocellaric acid
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid via intramol. titanium radical cyclization)
RN 220379-59-9 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



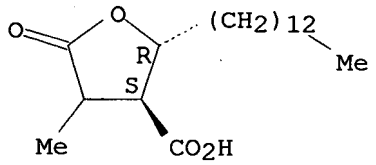
IT 249647-94-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid via intramol. titanium radical cyclization)

RN 249647-94-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

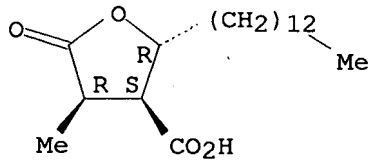


IT 249921-70-8P, (±)-Dihydroprotolichesterinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid via intramol. titanium radical cyclization)

RN 249921-70-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:811697 CAPLUS

DOCUMENT NUMBER: 130:168148

TITLE: Efficient total syntheses of (±)protolichesterinic acid and (±)rocellaric acid via tungsten-π-allyl complexes

AUTHOR(S): Chen, Ming-Jung; Liu, Rai-Shung

CORPORATE SOURCE: Department of Chemistry, National Tsing Hua University, Hsinchu, 30043, Taiwan

SOURCE: Tetrahedron Letters (1998), 39(51), 9465-9468
CODEN: TELEAY; ISSN: 0040-4039

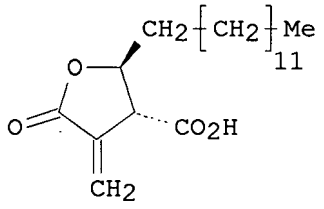
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

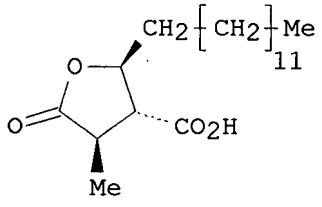
LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:168148

GI



I



II

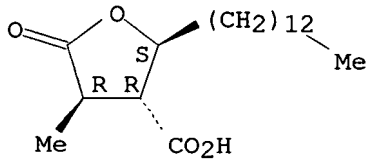
AB Total syntheses of racemic protolichesterinic acid (I) and rocellaric acid (II) were achieved with the use of tungsten-π-allyl complex in the key step. I and II were prepared in four and six steps resp. starting from readily available chloropropargyl derivs.

IT 220379-59-9P, (±)-Rocellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(total syntheses of (±)-protolichesterinic acid and (±)-rocellaric acid via tungsten-π-allyl complexes)

RN 220379-59-9 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:603556 CAPLUS

DOCUMENT NUMBER: 129:302486

TITLE: Synthesis of (±)-nephromopsinic acid

AUTHOR(S): Forster, Andrea; Fitremann, Juliette; Renaud, Philippe

CORPORATE SOURCE: Institut de Chimie Organique, Universite de Fribourg, Fribourg, 1700, Switz.

SOURCE: Tetrahedron Letters (1998), 39(39), 7097-7100
CODEN: TELEAY; ISSN: 0040-4039

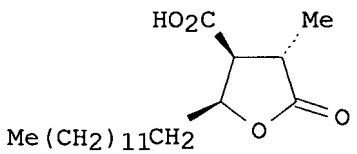
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:302486

GI



I

AB The preparation of (±)-nephromopsinic acid (I) form 7-oxabicyclo[2.2.1]hept-5-en-2-one is reported. The synthesis takes advantage of a previously

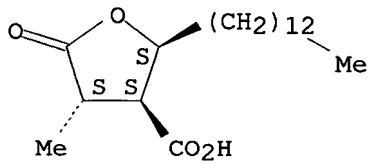
reported radical acyl migration. A remarkable iodide mediated cleavage of the bicyclic systems followed by the introduction of the γ-chain via a mixed Kolbe electrolysis are the key features of this approach. This strategy is expected to be of interest for the preparation of all kinds of paraconic acids with excellent control of the stereochem.

IT 214531-66-5P, (±)-Nephromopsinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of (±)-nephromopsinic acid)

RN 214531-66-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:169746 CAPLUS

DOCUMENT NUMBER: 128:204723

TITLE: Synthesis of (+)- and (-)-Phaseolinic Acid by Combination of Enzymic Hydrolysis and Chemical Transformations with Revision of the Absolute Configuration of the Natural Product

AUTHOR(S): Drioli, Sara; Felluga, Fulvia; Forzato, Cristina; Nitti, Patrizia; Pitacco, Giuliana; Valentin, Ennio

CORPORATE SOURCE: Dipartimento di Scienze Chimiche, Universita, Trieste, 34127, Italy

SOURCE: Journal of Organic Chemistry (1998), 63(7), 2385-2388
CODEN: JOCEAH; ISSN: 0022-3263

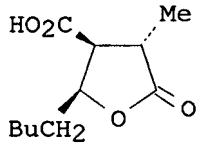
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

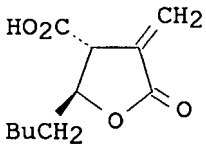
LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:204723

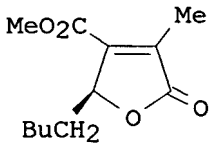
GI



I



II



III

AB Synthesis of both enantiomers of phaseolinic acid and on the determination of their absolute configurations via chemical and spectroscopic correlations is reported. The strategy was to correlate (-)-phaseolinic acid (I) with (-)-methylenolactocin (II) through the butenolide III.

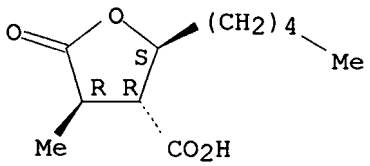
IT 203864-73-7P
RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(absolute configuration of phaseolinic acid enantiomers via stereoselective synthesis)

RN 203864-73-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 109667-12-1P 185246-65-5P

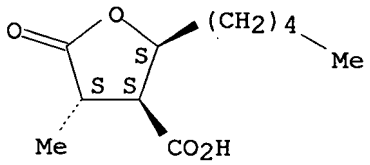
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(absolute configuration of phaseolinic acid enantiomers via stereoselective synthesis)

RN 109667-12-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

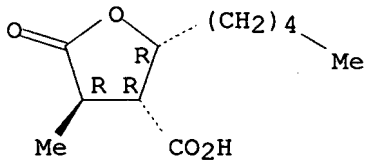
Absolute stereochemistry. Rotation (-).



RN 185246-65-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, [2R-(2α,3α,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 203514-35-6P, (±)-Phaseolinic acid

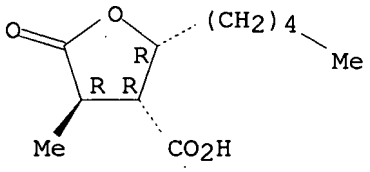
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(absolute configuration of phaseolinic acid enantiomers via stereoselective synthesis)

RN 203514-35-6 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

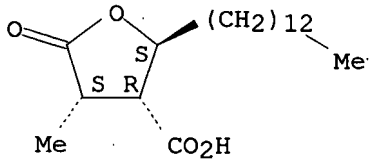
L5 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:521418 CAPLUS
DOCUMENT NUMBER: 127:176567
TITLE: Exerting face-stereoselective shielding: design of an enantiomeric pair of camphene-based oxazolidin-2-ones for use as recyclable chiral auxiliaries in asymmetric synthesis
AUTHOR(S): Cadogan, J. I. G.; Doyle, A. A.; Gosney, I.; Hodgson, P. K. G.; Thorburn, P.
CORPORATE SOURCE: Department of Chemistry, Imperial College of Science, Technology and Medicine, London, SW7 2AY, UK
SOURCE: Enantiomer (1997), 2(2), 81-98
CODEN: EANTE2; ISSN: 1024-2430
PUBLISHER: Gordon & Breach
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 17 refs. Preparative methodol. is described for access to a range of enantiomerically pure oxazolidin-2-ones by chemical elaboration of naturally-occurring compds. (terpenes, carbohydrates) via a stereospecific intramol. nitrene insertion reaction. The effectiveness and limitations of these reagents as chiral control elements in the form of their N-acyl derivs. for an array of asym. transformations is reported. In particular, the efficiency of a (+)-spiro-oxazolidin-2-one obtained from (-)-camphene is highlighted by the virtually complete stereoselection attained in such reactions as the Diels-Alder, conjugate addition, aldol, alkylation and acylation reactions. An added benefit to the spiro-oxazolidin-2-one is that its (-)-enantiomer is also readily accessible from (+)-camphene, thereby allowing preparative access to both enantiomeric products in a range of asym. manipulations. Both reagents are readily cleaved from the newly created chiral moieties and can be recycled. This exceptional quality of asym. induction imparted by the (+)-spiro-oxazolidin-2-one is highlighted by a concise synthesis of the tri-substituted lactone (-)-dihydroprotolichesterinic acid in 57% overall yield via consecutive stereo-controlled 1,4-conjugate addition and syn-aldol reactions.

IT 144356-39-8P, (-)-Dihydroprotolichesterinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(design of enantiomeric pair of camphene-based oxazolidin-2-ones for use as recyclable chiral auxiliaries in asym. synthesis)

RN 144356-39-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

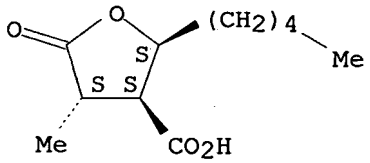
Absolute stereochemistry.



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:343886 CAPLUS
DOCUMENT NUMBER: 127:50457
TITLE: Asymmetric resolution of diastereomeric 4-ethoxycarbonyl-5-pentyl-γ-butyrolactones by crude PLE-mediated hydrolysis
AUTHOR(S): Drioli, Sara; Felluga, Fulvia; Forzato, Cristina; Nitti, Patrizia; Pitacco, Giuliana; Valentin, Ennio
CORPORATE SOURCE: Dipartimento di Scienze Chimiche, Universita di Trieste, via L. Giorgieri 1, Trieste, I-34127, Italy
SOURCE: Journal of Molecular Catalysis B: Enzymatic (1997), 3(1-4), 203-207
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:50457
AB Chemical reduction of di-Et 1-oxo-hexylsuccinate resulted in the formation of the corresponding cis and trans-disubstituted γ-butyrolactones. Both racemic diastereomers were resolved by means of lipolytic enzymes leading to the precursors of interesting natural products such as (-)-methylenolactocin and (-)-phaseolinic acid.
IT 109667-12-1P, (-)-Phaseolinic acid
RL: PNU (Preparation, unclassified); PREP (Preparation)
(asym. resolution of diastereomeric 4-ethoxycarbonyl-5-pentyl-γ-butyrolactones by crude PLE-mediated hydrolysis)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

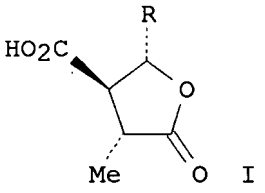
Absolute stereochemistry. Rotation (-).



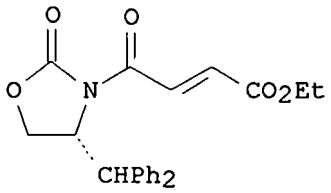
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:142049 CAPLUS
DOCUMENT NUMBER: 126:211956
TITLE: Regio- and stereocontrolled conjugate radical addition to a desymmetrized fumarate derivative: an efficient synthesis of (-)-nephrosteranic acid and (-)-roccellaric acid
AUTHOR(S): Sibi, Mukund P.; Ji, Jianguo
CORPORATE SOURCE: Dep. Chem., North Dakota State Univ., Fargo, ND, 58105-5516, USA
SOURCE: Angewandte Chemie, International Edition in English (1997), 36(3), 274-276
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: VCH
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:211956
GI



I



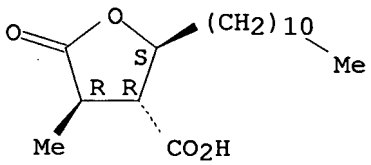
II

AB (-)-Nephrosteranic acid (I, R = C11H23) and (-)-roccellaric acid (I, R = C13H27) were prepared via high regio- and diastereoselective addition of the desymmetrized fumarate II with ClCH2I mediated by Samarium triflate.

IT 480-71-7P, (-)-Nephrosteranic acid 148676-05-5P, (-)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereocontrolled conjugate radical addition to a desymmetrized fumarate derivative in synthesis of (-)-nephrosteranic acid and (-)-roccellaric acid)

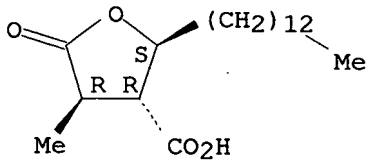
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:711181 CAPLUS
DOCUMENT NUMBER: 126:59779
TITLE: Enantioselective syntheses of (+)- and (-)-phaseolinic acid
AUTHOR(S): Jacobi, Peter A.; Herradura, Prudencio
CORPORATE SOURCE: Hall-Atwater Lab., Wesleyan Univ., Middletown, CT, 06459-0180, USA

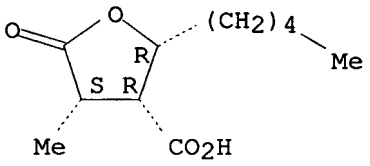
SOURCE: Tetrahedron Letters, (1996), 37(46), 8297-8300
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB (+)- And (-)-Phaseolinic acid have been prepared in an enantioselective fashion from (2S,3S,4R)-HO2CCHMeCH(C.tplbond.CH)CH(OCH2Ph)(CH2)4Me (I) by a three-step sequence involving lactonization, epimerization at C-3, and oxidative cleavage. I was obtained as a single enantiomer using a Nicholas-Schreiber reaction.

IT 185246-78-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective syntheses of (+)- and (-)-phaseolinic acid)

RN 185246-78-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, [2R-(2α,3α,4α)]- (9CI) (CA INDEX NAME)

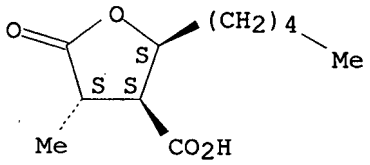
Absolute stereochemistry.



IT 109667-12-1P, (-)-Phaseolinic acid 185246-65-5P, (+)-Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective syntheses of (+)- and (-)-phaseolinic acid)

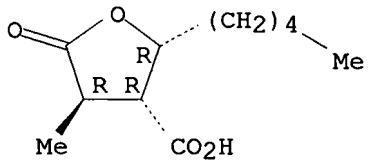
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



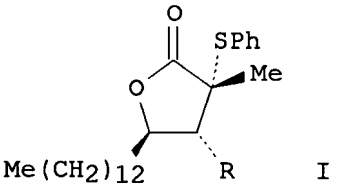
RN 185246-65-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, [2R-(2α,3α,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:501492 CAPLUS
DOCUMENT NUMBER: 125:167635
TITLE: Efficient Stereoselective Synthesis of the Enantiomers of Highly Substituted Paraconic Acids
AUTHOR(S): Martin, Tomas; Rodriguez, Carmen M.; Martin, Victor S.
CORPORATE SOURCE: Instituto Universitario de Bio-Organica Antonio Gonzalez, Universidad de La Laguna, La Laguna, 38206, Spain
SOURCE: Journal of Organic Chemistry (1996), 61(18), 6450-6453
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



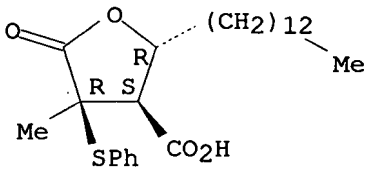
I

AB Rocellaric, protolichesterinic and dihydroprotolichesterinic acids were prepared stereoselectively via the common α-phenylthio-γ-lactone I [R = CH2CO2Me], obtained by a previously reported methodol. The described syntheses are general for this class of compds. The key steps are the conversion of the I [R = CH2CO2Me] to I [R = CO2H] with cleavage of one carbon, via I [R = CH(OH)CH2OH], and stereochem. controlled removal of the PhS group.

IT 180267-08-7P 180267-09-8P 180468-19-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of paraconic acids)

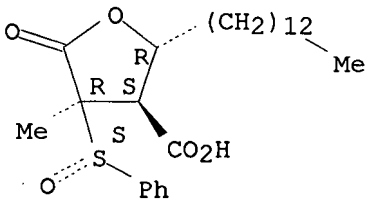
RN 180267-08-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-4-(phenylthio)-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



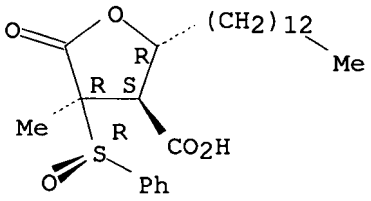
RN 180267-09-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-4-(phenylsulfinyl)-2-tridecyl-, [2R-[2α,3β,4β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



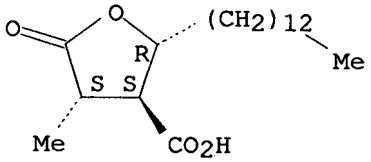
RN 180468-19-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-4-(phenylsulfinyl)-2-tridecyl-, [2R-[2α,3β,4β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



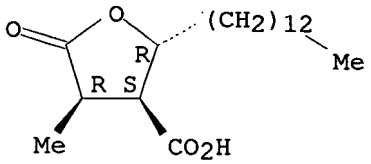
IT 19464-85-8P 19464-87-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of paraconic acids)
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



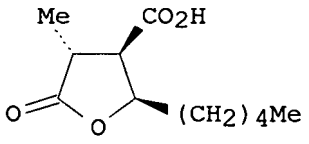
RN 19464-87-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

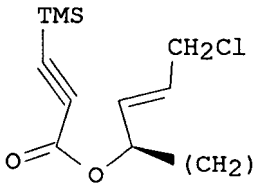


L5 ANSWER 18 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:465659 CAPLUS
DOCUMENT NUMBER: 125:195252
TITLE: Total synthesis of phaseolinic acid by enyne cyclization
AUTHOR(S): Zhang, Zhaoguo; Lu, Xiyan

CORPORATE SOURCE: Shanghai Inst. of Organic Chemistry, Chinese Acad. of Sci., Shanghai, 200032, Peop. Rep. China
SOURCE: Tetrahedron: Asymmetry (1996), 7(7), 1923-1928
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:195252
GI



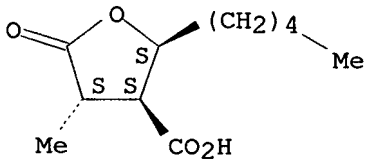
I



II

AB Enantiopure phaseolinic acid I was synthesized from (R)-4'-chloro-1'-n-pentyl-2'-butenyl 3-trimethylsilyl-2-propynoate II by palladium(II) catalyzed cyclization reaction as the key step.
IT 109667-12-1P, Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of phaseolinic acid via palladium(II) catalyzed enyne cyclization)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)-(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L5 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:274723 CAPLUS
DOCUMENT NUMBER: 125:10426
TITLE: Regio- and stereoselective functionalization of linear dicarboxylic acid derivatives. A sequential aldol-lactonization strategy for the synthesis of (-)-roccellaric acid, (-)-protolichesterinic acid, and (-)-methylenolactocin
AUTHOR(S): Sibi, Mukund P.; Deshpande, Prasad K.; La Loggia, Anthony J.
CORPORATE SOURCE: Dep. of Chemistry, North Dakota State Univ., Fargo, ND, 58105-5516, USA
SOURCE: Synlett (1996), (4), 343-345
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A regio- and stereoselective functionalization methodol. for linear dicarboxylic acids has been developed and applied in the synthesis of

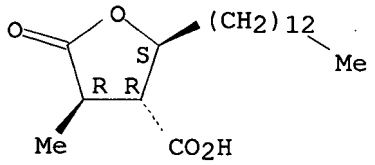
paraconic acid natural products. Using this strategy, (-)-roccellaric acid was prepared in 25% overall yield and 4 steps from a differentially functionalized succinate. The formal total synthesis of (-)-protolichesterinic acid and (-)-methylenolactocin was also accomplished starting from the differentially functionalized succinate.

IT 148676-05-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of paraconic acids)

RN 148676-05-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L5 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:746705 CAPLUS

DOCUMENT NUMBER: 123:143520

TITLE: Concise Syntheses of Natural γ-Butyrolactones, (+)-trans-Whisky Lactone, (+)-trans-Cognac Lactone, (-)-Methylenolactocin, (+)-Nephrosteranic Acid, and (+)-Roccellaric Acid Using Novel Chiral Butenolide Synthons

AUTHOR(S): Takahata, Hiroki; Uchida, Yasuhiro; Momose, Takefumi

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Toyama Medical Pharmaceutical University, Toyama, 930-01, Japan

SOURCE: Journal of Organic Chemistry (1995), 60(17), 5628-33
CODEN: JOCEAH; ISSN: 0022-3263

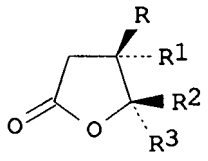
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

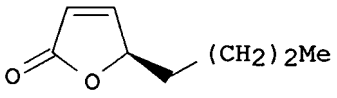
LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:143520

GI



I



II

AB Cis-4-Hydroxy-5-(iodomethyl)-4,5-dihydro-2(3H)-furanones I (R = OH, R1 = R3 = H, R2 = CH2I; R = R2 = H, R1 = OH, R3 = CH2I) were converted by cross-coupling with several Grignard-derived cuprates followed by benzoylation and base-induced elimination into new chiral butenolides, e.g., II. The sequential conjugate addition-quenching of these butenolides under complete stereocontrol provided several polysubstituted γ-butyrolactones including flavor components [(+)-trans-whisky lactone and (+)-trans-cognac lactone], the antitumor antibiotic lactone (-)-methylenolactocin, and lichen components [(+)-nephrosteranic acid and (+)-roccellaric acid].

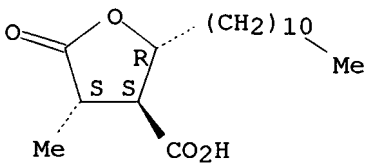
IT 70579-56-5P, (+)-Nephrosteranic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of whisky and cognac lactones, methylenolactocin, nephrosteranic and roccellaric acids)

RN 70579-56-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

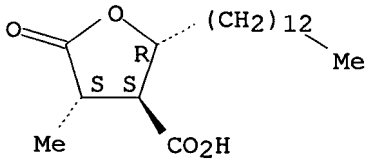


IT 19464-85-8P, (+)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of whisky and cognac lactones, methylenolactocin, nephrosteranic and roccellaric acids)

RN 19464-85-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



=> d his

(FILE 'HOME' ENTERED AT 09:23:46 ON 27 SEP 2007)

FILE 'REGISTRY' ENTERED AT 09:23:58 ON 27 SEP 2007
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 53 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:24:48 ON 27 SEP 2007
L4 73 S L3 FULL
L5 53 S L4 AND PY<2002
L6 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:29:07 ON 27 SEP 2007
L7 STRUCTURE UPLOADED
L8 5 S L7 FULL

FILE 'CAPLUS' ENTERED AT 09:29:29 ON 27 SEP 2007
L9 4 S L8 FULL

FILE 'STNGUIDE' ENTERED AT 09:29:55 ON 27 SEP 2007

FILE 'CAPLUS' ENTERED AT 09:32:24 ON 27 SEP 2007

FILE 'STNGUIDE' ENTERED AT 09:32:31 ON 27 SEP 2007

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	478.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-18.72

FILE 'CAPLUS' ENTERED AT 09:40:42 ON 27 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

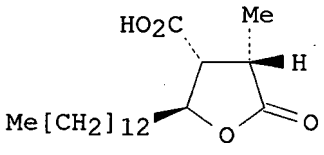
FILE COVERS 1907 - 27 Sep 2007 VOL 147 ISS 14
FILE LAST UPDATED: 26 Sep 2007 (20070926/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

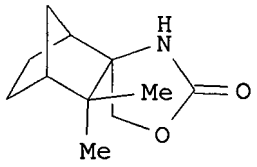
http://www.cas.org/infopolicy.html

=> d ibib abs hitstr l5 21-53

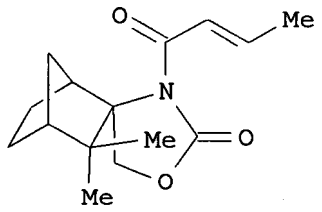
L5 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:597893 CAPLUS
DOCUMENT NUMBER: 123:83088
TITLE: A concise synthesis of (-)-dihydroprotolichesterinic acid via consecutive stereocontrolled 1,4-conjugate addition and syn-aldol condensation reactions
AUTHOR(S): Banks, Malcolm R.; Dawson, Ian M.; Gosney, Ian; Hodgson, Philip K. G.; Thorburn, Paul
CORPORATE SOURCE: Dep. of Chemistry, The University of Edinburgh, Edinburgh, EH9 3JJ, UK
SOURCE: Tetrahedron Letters (1995), 36(20), 3567-70
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:83088
GI



I



II



III

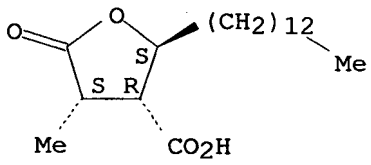
AB (-)-Dihydroprotolichesterinic acid I is synthesized in 6 steps and 57% overall yield by a strategy employing the camphene-derived chiral auxiliary II to construct the three contiguous stereogenic centers in consecutive stereocontrolled 1,4-conjugate addition of crotonyl imide III and syn-aldol reaction of tetradecanal with the vinylmagnesium bromide adduct of III.

IT 144356-39-8P, (-)-Dihydroprotolichesterinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dihydroprotolichesterinic acid via stereocontrolled conjugate addition and syn-aldol)

RN 144356-39-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

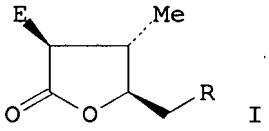
ACCESSION NUMBER: 1994:557410 CAPLUS
DOCUMENT NUMBER: 121:157410

TITLE: New entry to chiral butenolide synthons. Application to expeditious syntheses of (+)-nephrosteranic acid, (+)-trans-whisky lactone, and (+)-trans-cognac lactone

AUTHOR(S): Takahata, Hiroki; Uchida, Yasuhiro; Momose, Takefumi
CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Med. Pharmaceut. Univ., Toyama, 930-01, Japan

SOURCE: Tetrahedron Letters (1994), 35(24), 4123-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:157410

GI



I

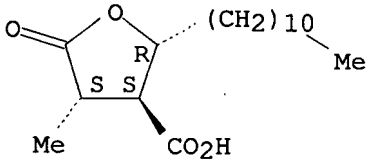
AB A new entry to chiral butenolide synthons starting with iodolactonization of the readily available, homochiral N-benzyl-N-methyl-3-hydroxy-4-pentenamide and its application to the syntheses of (+)-nephrosteranic acid I (R = C10H21, Nu, = CO2H, E = Me), (+)-trans-whisky lactone I (R = C3H7, Nu = Me, E = H), and (+)-trans-cognac lactone I (R = C4H9, Nu = Me, E = H) are described.

IT 70579-56-5P, (+)-Nephrosteranic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of)

RN 70579-56-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:603247 CAPLUS

DOCUMENT NUMBER: 119:203247

TITLE: Ring-opening aldol-type reaction of 2,2-dialkoxycyclopropanecarboxylic esters with carbonyl compounds. 3. The diastereoselective synthesis of 2,3,4-trisubstituted γ-lactones

AUTHOR(S): Shimada, Shigeru; Hashimoto, Yukihiko; Saigo, Kazuhiko

CORPORATE SOURCE: Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan

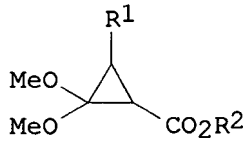
SOURCE: Journal of Organic Chemistry (1993), 58(19), 5226-34
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

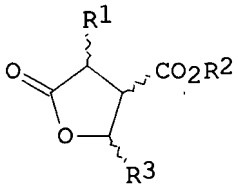
LANGUAGE: English

OTHER SOURCE(S): CASREACT 119:203247

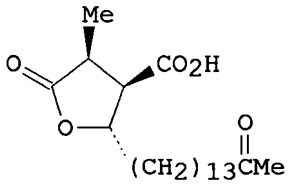
GI



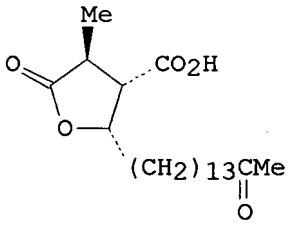
I



II



III



IV

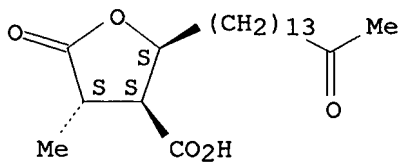
AB The Lewis acid-promoted reaction of 3-alkyl-2,2-dialkoxycyclopropanecarboxylic esters I (R1 = R2 = Me, Et; R1 = Me, R2 = Et, CMe3; R1 = CHMe2, R2 = Et) with R3CHO (R3 = cyclohexyl, n-heptyl, CHMe2, CMe3, Ph, PhCH2CH2) to give 2,3,4-trisubstituted γ-lactones II (trans-trans, trans-cis, cis-trans, cis-cis) was investigated. The diastereoselectivity of this reaction is highly dependent on the catalyst employed. Thus while the ZrCl4-promoted reaction gave (2α,3α,4β)-trisubstituted γ-lactones in good yields with excellent selectivity, the SnBr4-promoted reaction was moderately selective for (2α,3α,4α)-trisubstituted γ-lactones. The present reaction was applied to the synthesis of (+)589- and (-)589-dihydropertusaric acid (III). Comparison of the spectroscopic and phys. data of synthetic III with those of a 4-alkyl-3-carboxy-2-Me γ-lactone isolated from the lichen Pertusaria albescens revealed that the relative stereochem. of the natural γ-lactone was not (2β,3β,4α), as reported by Huneck and his co-workers, but rather (2β,3α,4α); i.e., the natural γ-lactone was not (-)589-dihydropertusaric acid III, but (-)589-pertusarinic acid (IV).

IT 101899-68-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 101899-68-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2S,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L5 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:495208 CAPLUS

DOCUMENT NUMBER: 119:95208

TITLE: First asymmetric synthesis of (+)- and (-)-roccellaric acid and dihydroprotolichesterinic acid

AUTHOR(S): Mulzer, Johann; Salimi, Nabiollah; Hartl, Hans

CORPORATE SOURCE: Inst. Org. Chem., Freie. Univ. Berlin, Berlin,

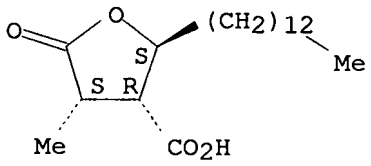
W-1000/33, Germany
SOURCE: Tetrahedron: Asymmetry (1993), 4(3), 457-71
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Stereocontrolled syntheses of the title compds. from (R)-2,3-isopropylideneglyceraldehyde, (S)-O-tetrahydropyranyllactaldehyde and 1,2:5,6-di-O-isopropylidene-α-D-glucofuranose (diacetone-D-glucose) are described.

IT 144356-39-8P 148676-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

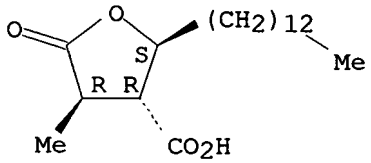
RN 144356-39-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

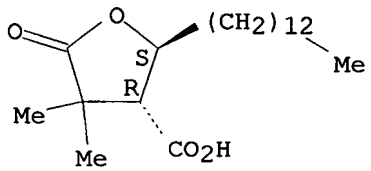
Absolute stereochemistry. Rotation (-).



IT 148676-08-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

RN 148676-08-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4,4-dimethyl-5-oxo-2-tridecyl-, (2S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

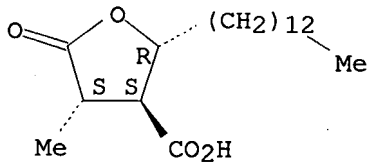


IT 19464-85-8P 19464-87-0P 149207-16-9P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of)

RN 19464-85-8 CAPLUS

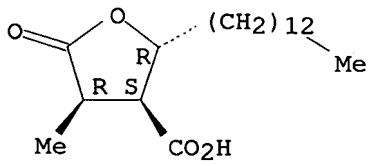
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



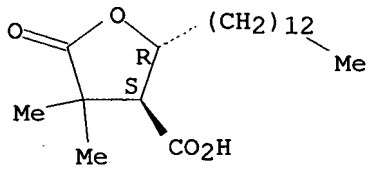
RN 19464-87-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

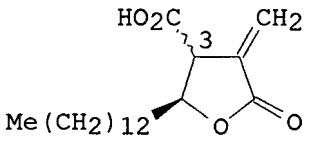


RN 149207-16-9 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4,4-dimethyl-5-oxo-2-tridecyl-, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 25 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:630101 CAPLUS
DOCUMENT NUMBER: 117:230101
TITLE: Contribution to the chemistry of proto- and allo-protolichesterinic acids
AUTHOR(S): Huneck, Siegfried; Takeda, Reiji
CORPORATE SOURCE: Inst. Pflanzenbiochem., Halle/Saale, D-O-4050, Germany
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1992), 47(6), 842-54
CODEN: ZNBSEN; ISSN: 0932-0776
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

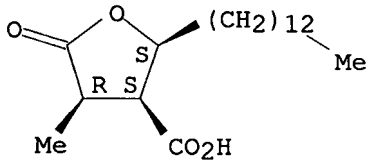


I, 3?
II, 3?

AB The isolation and spectroscopic characterization of (-)-allo-protoichesterinic acid (I) from Cetraria komarovii is described. Protolichesterinic acid (II) and I were transformed into numerous nitrogen-containing derivs. and the isomerization of the dihydro acids was investigated.

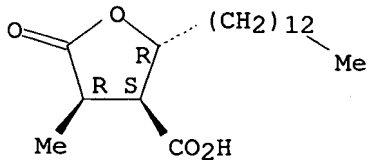
IT 493-45-8
RL: BIOL (Biological study)
(of Cetraria komarovii)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



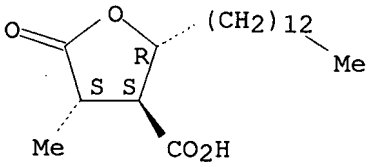
IT 19464-87-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 19464-87-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



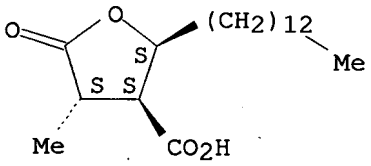
IT 19464-85-8P 133695-37-1P 144356-39-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



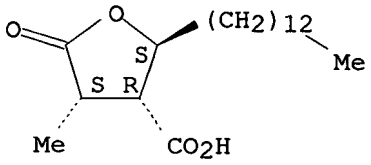
RN 133695-37-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3α,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

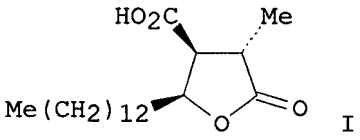


RN 144356-39-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:247032 CAPLUS
DOCUMENT NUMBER: 114:247032
TITLE: Highly Felkin-Anh selective Hiyama additions of chiral allylic bromides to aldehydes. Application to the first synthesis of nephromopsinic acid and its enantiomer
AUTHOR(S): Mulzer, Johann; Kattner, Lars; Strecker, Achim R.; Schroeder, Christian; Buschmann, Juergen; Lehmann, Christian; Luger, Peter
CORPORATE SOURCE: Inst. Org. Chem., Freie Univ. Berlin, Berlin, D-1000/33, Germany
SOURCE: Journal of the American Chemical Society (1991), 113(11), 4218-29
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:247032
GI



I

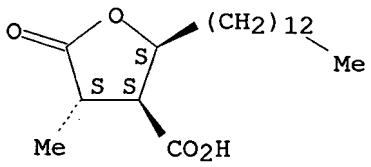
AB The Cr(II)-mediated addition (Hiyama reaction) of chiral allylic bromides to achiral and chiral aldehydes proceeds with high Felkin-Anh selectivity with respect to the stereocenter at C-γ in the bromide. Double stereodifferentiation expts. show that the bromide is the stereodominating component in the addition The methodol. was applied to the first synthesis of nephromopsinic acid (I), found in the lichen species Nephromopsis stracheyi, and its enantiomer. Crystal structures are reported for two of the adducts.

IT 133695-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
((-)-Nephromopsinic acid; total synthesis of)

RN 133695-37-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3α,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

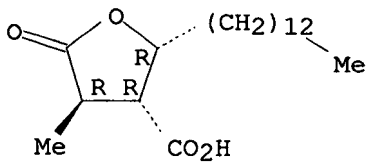


IT 133695-45-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)

RN 133695-45-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:88475 CAPLUS

DOCUMENT NUMBER: 112:88475

TITLE: Nonsymmetric spherulites: nephrasteranic acid

AUTHOR(S): Prasad, P. B. V.; Prasad, N. Durga

CORPORATE SOURCE: Dep. Phys., Gov. Polytech., Warangal, 506007, India

SOURCE: Crystal Research and Technology (1989), 24(10), K183-K186
CODEN: CRTEDF; ISSN: 0232-1300

DOCUMENT TYPE: Journal

LANGUAGE: English

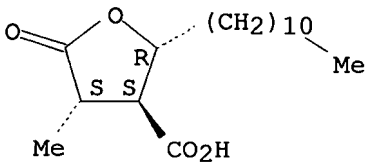
AB Sym. and asym. spherulitic crystallization of nephrasteranic acid is discussed. The extent of asymmetry observed in the present case is employed to make certain qual. estns.

IT 70579-56-5, Nephrasteranic acid
RL: PRP (Properties)
(crystallization of nonsym. spherulites of)

RN 70579-56-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 28 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:489797 CAPLUS

DOCUMENT NUMBER: 109:89797

TITLE: Lichen constituents. Part 149: Components of some lichens from Mongolia

AUTHOR(S): Huneck, S.; Tuja, D.; Cogt, U.

CORPORATE SOURCE: Inst. Biochem., Akad. Wiss. DDR, Halle/Saale, Ger. Dem. Rep.

SOURCE: Pharmazie (1988), 43(5), 371-2
CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: German

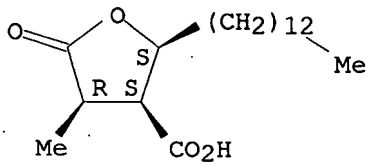
AB Aspicilia vagans From the Mongolian Altai contained triglycerides and phytosterols. Cetraria tilesii Contained pinastric, (-)-usnic, and vulpinic acids, Dactylina madreporiformis contained (+)-usnic and (-)-nephromopsic acids, Rhizoplaca baranowii contained (-)-usnic and psoromic acids, triglycerides, and phytosterols, and Xanthoria elegans contained parietin.

IT 493-45-8
RL: BIOL (Biological study)
(in lichens from Mongolian Altai)

RN 493-45-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

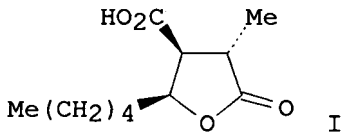
ACCESSION NUMBER: 1987:473910 CAPLUS

DOCUMENT NUMBER: 107:73910

TITLE: Structure and stereochemistry of phaseolinic acid: a new acid from Macrophomina phaseolina

AUTHOR(S): Mahato, Shashi B.; Siddiqui, Kazi A. I.; Bhattacharya,

Gautam; Ghosal, Tapasree; Miyahara, Kazumoto; Sholichin, Mochammad; Kawasaki, Toshio
CORPORATE SOURCE: Indian Inst. Chem. Biol., Calcutta, 700 032, India
SOURCE: Journal of Natural Products (1987), 50(2), 245-7
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

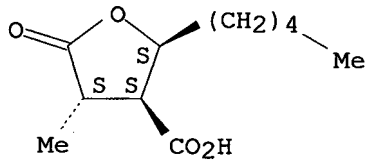
AB A new acid designated phaseolinic acid (I) was isolated from the culture filtrate of M. phaseolina. The structure of I was determined by its IR, 1H NMR, and mass spectra and single crystal x-ray crystallog. The absolute configuration of I was 2R,3R,4R.

IT 109667-12-1
RL: BIOL (Biological study)
(from Macrophomina phaseolina, isolation and structure determination of)

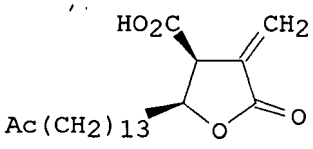
RN 109667-12-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

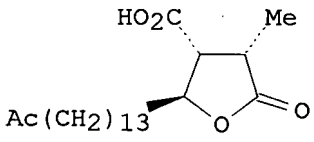
Absolute stereochemistry. Rotation (-).



L5 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:183270 CAPLUS
DOCUMENT NUMBER: 104:183270
TITLE: Lichen substances. Part 144. (-)-Allo-pertusaric acid and (-)-dihydropertusaric acid from the lichen Pertusaria albescens
AUTHOR(S): Huneck, Siegfried; Toensberg, Tor; Bohlmann, Ferdinand
CORPORATE SOURCE: Inst. Plant Biochem., Ger. Acad. Sci., Halle/Saale, 4010, Ger. Dem. Rep.
SOURCE: Phytochemistry (Elsevier) (1986), 25(2), 453-9
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

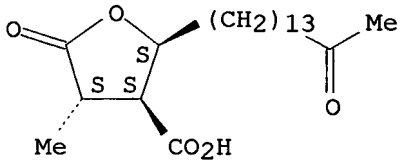
AB The structures of 2 γ-lactone carboxylic acids from the lichen P. albescens, (-)-allo-pertusaric acid (I) and (-)-dihydropertusaric acid (II), were elucidated by spectroscopic and chemical methods. From P. ophthalmiza, taraxerone and a mixture of long-chain aliphatic alcs. and fatty acids were isolated.

IT 101899-68-7
RL: BIOL (Biological study)
(of Pertusaria albescens, structure of)

RN 101899-68-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2S,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

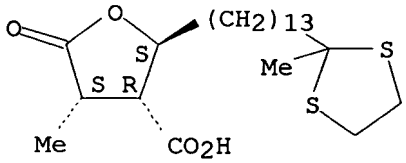


IT 101899-75-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation and desulfurization of)

RN 101899-75-6 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-[13-(2-methyl-1,3-dithiolan-2-yl)tridecyl]-5-oxo-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

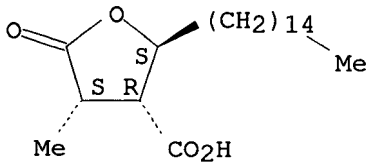


IT 101899-66-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)

RN 101899-66-5 CAPLUS

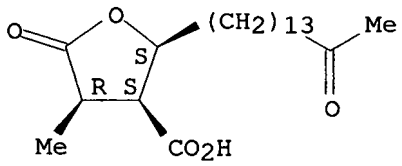
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentadecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



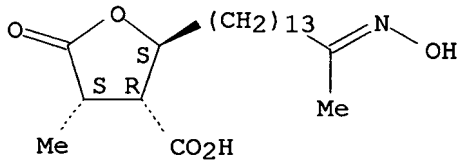
IT 101899-63-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with diazomethane)
RN 101899-63-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, [2S-(2α,3α,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 101899-69-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 101899-69-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[14-(hydroxyimino)pentadecyl]-4-methyl-5-oxo-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



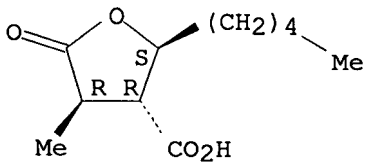
L5 ANSWER 31 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:592767 CAPLUS
DOCUMENT NUMBER: 103:192767
TITLE: Metabolites of the higher fungi. Part 2. 2-Butyl-3-methylsuccinic acid and 2-hexylidene-3-methylsuccinic acid from xylariaceous fungi
AUTHOR(S): Anderson, John R.; Edwards, Raymond L.; Whalley, Anthony J. S.
CORPORATE SOURCE: Sch. Chem., Univ. Bradford, Bradford, BD7 1DP, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (7), 1481-5
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The diacid (+)-erythro-HO2CCHMeCHBuCO2H was isolated from Hypoxylon illitum. (+)-(E)-HO2CCHMeC(CO2H):CH(CH2)4Me [(+)-(E)-I] was isolated from

H. deustum, (-)-(E)-I from Xylaria polymorpha, X. longipes, and Poronia piliformis, and the racemic (E)-I was obtained from X. mali and X. hypoxylon. The structures and configurations of these compds. were determined by spectral and synthetic methods.

IT 98985-82-1P 98985-83-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

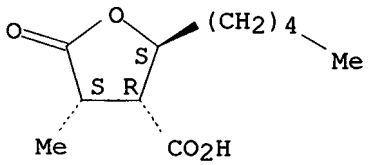
RN 98985-82-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2α,3β,4α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



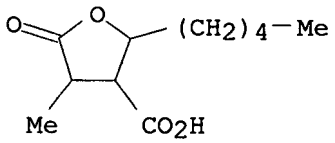
RN 98985-83-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2α,3β,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 98985-77-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 98985-77-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl- (9CI) (CA INDEX NAME)



L5 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1984:607615 CAPLUS
DOCUMENT NUMBER:	101:207615
TITLE:	Ecological and chemical investigations of lichens from South Georgia and the maritime Antarctic
AUTHOR(S):	Huneck, S.; Sainsbury, M.; Rickard, T. M. A.; Smith, R. I. Lewis
CORPORATE SOURCE:	Inst. Plant Biochem., Acad. Sci. GDR, Halle/Saale, GDR-401, Ger. Dem. Rep.
SOURCE:	Journal of the Hattori Botanical Laboratory (1984), 56, 461-80

CODEN: JHBLAI; ISSN: 0073-0912
DOCUMENT TYPE: Journal
LANGUAGE: English

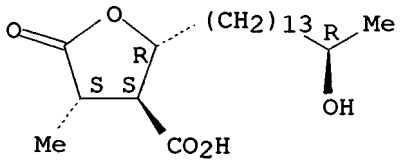
AB Compds. of a possible chemotaxonomic importance found in 20 lichen taxa, which were collected in 5 localities of South Georgia and in the maritime Antarctic, are described. Parietin, fumarprotocetraric acid, atranorin, arthothelin, barbatolic acid , zeorin,, protocetraric acid,, calycin, 2α-acetoxystictane-3β,22α-diol, stictane-2α,3β,22α-triol, pseudocyphellarin A and B, (-)-usnic acid, stictic acid, constictic acid, 7β-acetoxyhopane-22-ol, hopane-15α,22-diol, (+)-usnic acid, rhizocarpic acid, psoromic acid, thamnolic acid, sphaerophorin, lobaric acid, , murolic acid, neodihydromurolic acid, and salazinic acids were found in Caloplaca regalis, Cladonia gracilis, C. pycnoclada, C. rangiferina, Haematomma erythromma, Himantormia lugubris, Lecidella bullata, Pertusaria dactylina, Pseudocyphellaria endochrysa, P. freycinetti, Ramalina terebrata, Rhizocarpon geographicum, Sphaerophorus globosus, Stereocaulon glabrum, Usnea antarctica, U. fasciata, and U. sulphurea, in a chemotaxonomically characteristic manner. In Umbilicaria antarctica, gyrophoric acid, a mixture of sterols, trilinolein and other triglycerides with oleic, palmitic, and palmitoleic acids were found. U. decussata Contained a mixture of triglycerides almost identical with that in U. antarctica. In Leptogium menziesii, 14 compds., none of which could be identified, were found in the ether exts. The ecol. of each taxon is given.

IT 70579-57-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of lichens from South Georgia and maritime Antarctic)

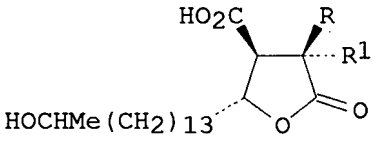
RN 70579-57-6 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4S)- (9CI) (CA INDEX NAME)

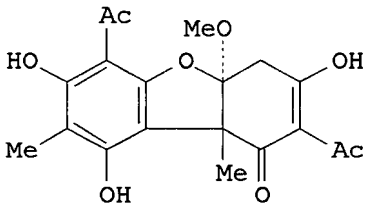
Absolute stereochemistry.



L5 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:607428 CAPLUS
DOCUMENT NUMBER: 91:207428
TITLE: Recent results in the chemistry of lichen substances
AUTHOR(S): Huneck, Siegfried
CORPORATE SOURCE: Inst. Plant Biochem., Ger. Acad. Sci., Halle/Saale, DDR-401, Ger. Dem. Rep.
SOURCE: Symp. Pap. - IUPAC Int. Symp. Chem. Nat. Prod., 11th (1978), Volume 4, Issue Part 1, 197-206.
Editor(s): Marekov, N.; Ognyanov, I.; Orahovats, A.
Izd. BAN: Sofia, Bulg.
CODEN: 41RTAX
DOCUMENT TYPE: Conference
LANGUAGE: English
GI



I, $RR^1=CH_2$
II, R=H, R^1=Me



III

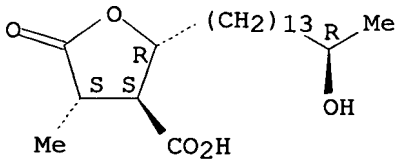
AB In studies on lichen substances, the structures of 2 γ-lactone carboxylic acids, 2 δ-lactone carboxylic acids, 3 chloroxanthones, and a new dibenzofuran derivative were elucidated. Lecanora muralis Yielded murolic (I) and neodihydromurolic (II) acids, along with (+)-usnic acid, psoromic acid, zeorin, and leucotylin. I and II were also found in L. melanophthalma and L. rubins. The latter species also contained (-)-pseudoplacodiolic acid (III). Pertusaria aleianta Contained a mixture of chloroxanthones: 2,5-dichlorolichexanthone, 2,4-dichlorolichexanthone, and 2,4,5-trichlorolichexanthone. Acarospora chlorophane Contained acaranoic and acarenoic acids.

IT 70579-57-6
RL: BIOL (Biological study)
(from Lecanora species)

RN 70579-57-6 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:435683 CAPLUS
DOCUMENT NUMBER: 91:35683
TITLE: Neodihydromurol and murolic acid, two new γ-lactonecarboxylic acids from Lecanora muralis
AUTHOR(S): Huneck, Siegfried; Schreiber, Klaus; Hoefle, Gerhard; Snatzke, Guenther
CORPORATE SOURCE: Inst. Biochem., DAW, Halle/Saale, DDR-401, Ger. Dem. Rep.
SOURCE: Journal of the Hattori Botanical Laboratory (1979), 45, 1-23
CODEN: JHBLAI; ISSN: 0073-0912
DOCUMENT TYPE: Journal
LANGUAGE: German

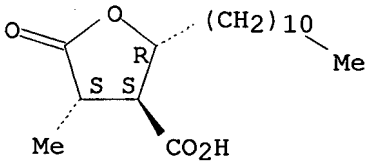
AB Two new aliphatic hydroxy γ-lactone carboxylic acids, (+)-neodihydromurolic acid and (+)-murolic acid, were isolated from the lichens Lecanora muralis, L. melanophthalma, and L. rubina. Spectroscopical and chemical data led to the following structures:

(+)-neodihydromurolic acid, (+)-2(S)-methy-3(S)-carboxy-4(R),18(R)-dihydroxynonadecan-1→4-olide (I); and (+)-murolic acid, (+)-2-methylen-3(S)-carboxy-4(R),18(R)-dihydroxynonadecan-1→4-olide (II). The absolute configurations of (+)-nephrosteranic acid, (-)-alloprotolichesterinic acid, and (+)-nephrosterinic acid were established.

IT 70579-56-5P 70579-60-1P 70579-70-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

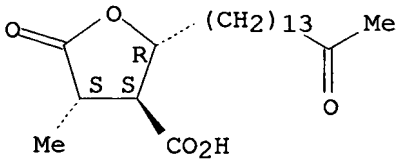
RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



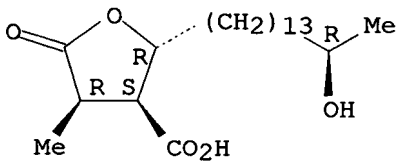
RN 70579-60-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2R,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 70579-70-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4R)- (9CI) (CA INDEX NAME)

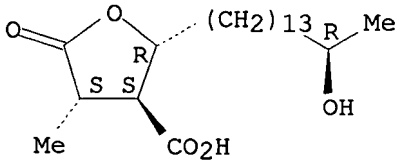
Absolute stereochemistry.



IT 70579-57-6
RL: BIOL (Biological study)
(Lecanora lactonecarboxylic acid)

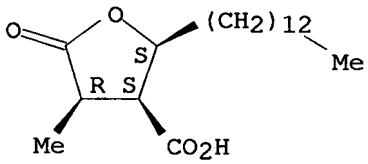
RN 70579-57-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 35 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:77124 CAPLUS
DOCUMENT NUMBER: 70:77124
TITLE: Naturally occurring lactones and lactams. I. Absolute configuration of ranunculin, lichesterinic acid, and some lactones related to lichesterinic acid
AUTHOR(S): Boll, Per M.
CORPORATE SOURCE: Univ. Copenhagen, Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1968), 22(10), 3245-50
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English
AB N.M.R. spectra have confirmed the provisional structure of ranunculin. Circular dichroism data allowed the assignment of the configuration of its aglucone to be 4S. As a result of the circular dichroism work, it was also possible to allocate configurations to the following lichen lactones: (S)-(-)-lichesterinic acid, (3R,4S)-(-)-protolichesterinic acid, (3S,4S)-(-)-alloprotolichesterinic acid, and (2R,3S,4S)-nephromopsic acid.
IT 493-45-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 36 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:49000 CAPLUS
DOCUMENT NUMBER: 68:49000
ORIGINAL REFERENCE NO.: 68:9455a,9458a
TITLE: Lichen constituents. XXXV. Chilean lichens. 14. Components of Rocellaria % mollis and the structure and absolute configuration of roccellaric acid
AUTHOR(S): Huneck, Siegfried; Follmann, Gerhard
CORPORATE SOURCE: Tech. Univ. Dresden, Tharandt, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, Biochemie, Biophysik, Biologie (1967), 22(6), 666-70
CODEN: ZENBAX; ISSN: 0044-3174
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.

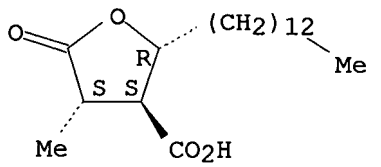
AB R. mollis (77 g.) was extracted with Et2O 10 hrs., the extract shaken with aqueous NaHCO3 solution, which was acidified and again extracted with Et2O. The residue on evaporation of this last Et2O extract recrystd. from HOAc and then from MeOH yielded 1.75% roccellaric acid (I), m. 110-11°, [α]20D 35° (c 1.73, CHCl3); Me ester m. 40-1°, [α]20D 25° (c 1.53, CHCl3). Protolichesteric acid (II) was prepared by extracting Cetraria islandica with Et2O, extracting the ether extract with aqueous NaHCO3 acidifying, and extracting with Et2O; m. 107-8°, [α]20D 15° (c 4.73, CHCl3). II was converted into (+)-dihydroprotolichesteric acid (III) by hydrogenation with Pd-charcoal in HOAc, m. 104-6°; Me ester m. 50-1°, [α]20D 60° (c 1.76, CHCl3). III was reduced with 0.0428 g. Na in 9.6 ml. MeOH, 1 hr. on a steam bath, the mixture diluted with 20 ml. water, acidified with 10% H2SO4 and extracted with Et2O to give the Me ester (IV) of (+)-neo-dihydroprotolichesteric acid (V). Saponification of IV with NaOH in MeOH 5 days at room temperature gave V, m. 110-11°, [α]20D 38° (c 1.77, CHCl3). Comparison of V and IV were identical with I and its Me ester, resp. Reduction with LiAlH4 of the Me ester of I gave needles m. 59-61°, [α]20D 10° (c 1.29, CHCl3). The residue of R. mollis from the extraction with Et2O was extracted with acetone, the extracted residue extracted with water and the water extract evaporated Recrystn. from EtOH yielded 0.02% meso-erythritol, m. 119-20°. The residue from the extraction with water was dried and recrystd. from acetone, yielding 1.96% mollin, m. 270-1° (decomposition); acetyl derivative m. 208-9° (MeOH). The acetone mother liquor from the crystallization of mollin was concentrated and the residue recrystd. from HOAc to yield 1.3% roccellin, m. 206-7°, acetyl derivative m. 210°. Mollin and roccellin are new compds. Study of the O.R.D. curve of (+)-neo-dihydroprotolichesteric acid Me ester and its hydrogenation product and reference to the literature on similar compds., e.g. roccellic acid whose configuration was worked out by Akermark established the configuration I for roccellaric acid, 4-carboxy-3-methyl-2-oxo-5-tridecyltetrahydrofuran.

IT 19464-85-8P
RL: PREP (Preparation)
(from Roccellaria mollis)

RN 19464-85-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

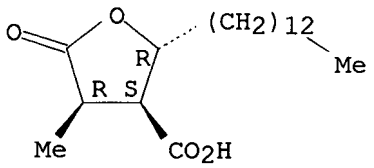


IT 19464-87-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19464-87-0 CAPLUS

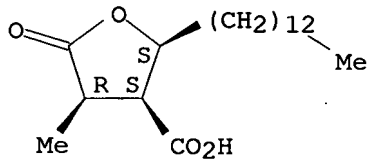
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:497597 CAPLUS
DOCUMENT NUMBER: 67:97597
ORIGINAL REFERENCE NO.: 67:18339a,18342a
TITLE: Lichens. IV. Thin-layer chromatography of lichen substances
AUTHOR(S): Santesson, Johan
CORPORATE SOURCE: Univ. Uppsala, Uppsala, Swed.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1967), 21(5), 1162-72
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 67: 51056p. The thin-layer chromatography on precoated plates of >80 lichen substances is described. 32 references.
IT 493-45-8
RL: ANT (Analyte); ANST (Analytical study)
(thin-layer chromatog. of)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 38 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:475198 CAPLUS
DOCUMENT NUMBER: 65:75198
ORIGINAL REFERENCE NO.: 65:14079a-b
TITLE: Lichens. II. Thin-layer chromatography of aliphatic lichen acids
AUTHOR(S): Bendz, Gerd; Santesson, Johan; Tibell, Leif
CORPORATE SOURCE: Univ. Uppsala, Swed.
SOURCE: Acta Chemica Scandinavica (1966), 20(4), 1180-1
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 64, 13073b. Aliphatic lichen acids were separated by thin layer chromatog. on silica gel HF, by using 40 mg. bromcresol green in 100 mL. 0.01N NaOH as the detection spray. Rf values were tabulated.Rf + 100 in solvent system, A, B, C, D; Caperatic acid, 03, 02, 01, 11; Lichesterinic acid, 73, 32, 56, X; Nephromopsinic acid, 82, 32, 54, X; Nephrosteranic acid, 82, 31, 55, X; Nephrosterinic acid, 61, 22, 43, X, Norrangiformic acid, 04, 03, 03, 49; Acaranoic acid, 68, 26, 42, X;

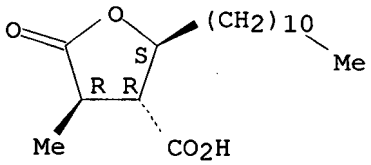
Acarenoic acid, 48, 17, 30, X; Protolichesterinic acid, 61, 23, 43, X; Rangiformic acid, 50, 10, 36, 66; Roccellic acid, 91, 24, 60, X; X indicates that the acid travels with the secondary front; the solvents were: (A) ether-butyric acid 20:1, (B) CHCl3-propionic acid 20:1, (C) iso-Pr ether-propionic acid 20: 1, (D) CHCl3-HOAc 5:1.

IT 480-71-7, Nephrosteranic acid 493-45-8, Nephromopsinic acid
(chromatog. of)

RN 480-71-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

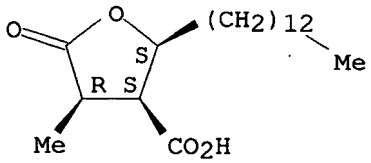
Absolute stereochemistry. Rotation (-).



RN 493-45-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:113136 CAPLUS

DOCUMENT NUMBER: 52:113136

ORIGINAL REFERENCE NO.: 52:19935g-i,19936a-i,19937a-h

TITLE: The synthesis of dl-protolichesterinic acid

AUTHOR(S): Van Tamelen, Eugene E.; Bach, Shirley Rosenberg

CORPORATE SOURCE: Univ. of Wisconsin, Madison

SOURCE: Journal of the American Chemical Society (1958), 80, 3079-86
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:113136

AB Me dl-dihydroprotolichesterinate (180 mg.), 0.024 g. Na, and 5.5 cc. MeOH refluxed 1 hr., poured into H2O, acidified with NaHSO4, extracted with Et2O, the extract worked up, the residue (0.129 g.) dissolved in 7 cc. MeOH, the solution treated with 1 cc. H2O containing 0.0304 g. NaOH, kept 5 days at room temperature, diluted with H2O, acidified with NaHSO4, and the precipitate recrystd. from glacial AcOH, washed with petr. ether, and recrystd. again from MeOH yielded 0.056 g. neodihydroprotolichesterinic acid (I), platelets, m. 97-8° (all m.ps. are corrected) I with CH2N2 gave the Me ester, m. 38-9° (uncor.). Me dl-isodihydroprotolichesterinate (0.31 g.) and 10.5 cc. absolute MeOH refluxed 5.5 hrs. with 0.00419 g. Na, treated with 1 cc. H2O, refluxed 6.5 hrs., cooled, diluted with H2O, acidified with NaHSO4, extracted with Et2O, the extract worked up, and the residue extracted with cold petr.

ether left 0.070 g. I. $C_{13}H_{27}COCH_2CO_2Me$ (II) (5 g.) and 2.9 g. powdered NaI added to 0.41 g. Na in 10 cc. absolute MeOH, the mixture treated with cooling during 10 min. with 3.0 g. $BrCH_2CO_2Et$, kept 2 days at room temperature, filtered, the residue washed with H_2O, the filtrate poured into H_2O, acidified and extracted with Et_2O, and the extract worked up yielded 2.53 g. dialkylation product, $C_{25}H_{44}O_7$, m. 42-3°. II (10 g.), 100 cc. dry C_6H_6, and 10 g. pyrrolidine, b. 86.5-87° refluxed 9 hrs. with the azeotropic removal of about 0.8 cc. H_2O and evaporated gave 11.5 g. pyrrolidine enamine (III) of II, yellow liquid. III (11.5 g.), 100 cc. absolute MeOH, and 5.85 g. $BrCH_2CO_2Et$ refluxed 29 hrs., and stirred overnight with 20 cc. H_2O, the aqueous layer extracted with Et_2O, and the combined organic layer and extract evaporated gave 10 g. brown oily $C_{13}H_{27}COCH(CO_2Me)CH_2CO_2Et$ (IV); a 10-g. portion in 50 cc. absolute MeOH treated with 8 cc. 1.0M $NaBH_4$ in MeOH, allowed to stand 3 days, treated again with 11 cc. $NaBH_4$ solution, allowed to stand 3 hrs., poured into H_2O, acidified with $NaHSO_4$, and extracted with Et_2O, the extract washed, dried, and evaporated, the residual yellow oil dissolved with 7 g. KOH in 110 cc. 90% MeOH, allowed to stand 1 day at room temperature, cooled, filtered, the residue acidified with 5% HCl, digested 1 hr. at 70°, kept several hrs. at room temperature, filtered, dried (5.1 g.), and recrystd. from C_6H_6 yielded 4.8 g. 3-carboxy-4-oxoheptadecanoate (V), m. 80-3°. V (1 g.) treated with CH_2N_2 in Et_2O and evaporated yielded 1.03 g. β-carbomethoxy-γ-tridecyl-γ-butyrolactone (VI), m. 68-70° (MeOH). $(EtO)_2CO$ (80 g.) and 8.6 g. butyrolactone refluxed at 125 mm., treated during 1 hr. with 2.39 g. Na in 56 cc. absolute EtOH while removing the EtOH simultaneously with the addition, the residual pale yellow, gelatinous mass poured into 60 cc. glacial AcOH and ice and extracted with 50 cc. Et_2O, and the extract worked up yielded 4.1 g. α-carbethoxy-γ-butyrolactone(VII), b0.5, 106-9°. VII in EtOH treated with excess liquid NH_3 gave $HO(CH_2)_2CH(CONH_2)_2$, m. 152.5-53° (EtOH). VI (3 g.) and 7.55 g. $(EtO)_2CO$ treated dropwise during 1 hr. with stirring under reflux at 125 mm. with 0.212 g. Na in 5.6 cc. absolute EtOH while removing the EtOH continuously, the resulting slush poured into 6 cc. glacial AcOH and ice and extracted with Et_2O, and the extract worked up yielded 3.4 g. light red oil; a 0.79-g. portion chromatographed on 12 g. silicic acid did not give the desired carbethoxylation product; a 2.37-g. portion in 20 cc. MeOH containing 1.27 g. KOH kept 5 days at room temperature, acidified with 5% HCl, filtered, and the residue washed with H_2O, dried, and extracted with ligroine (b. 60-8°) left 1.4 g. material $C_{18}H_{32}O_4$, m. 133-5°. $C_{13}H_{27}CH{:}CHCO_2H$ (VIII), m. 47-9° (aqueous EtOH), was prepared by the method of Myers (C.A. 46, 1438g) and separated in 45% yield from the by-product $C_{14}H_{29}CH(OH)CO_2H$ by extracting the crude mixture with petr. ether at room temperature, filtering, cooling to 0°, filtering again, evaporating, and recrystg. the residue from aqueous MeOH. VIII (5 g.) in 50 cc. Et_2O treated with CH_2N_2 in Et_2O until the yellow color persisted for 5 min. and evaporated on the steam bath gave 5.3 g. Me ester (IX) of VIII. trans-VIII (1.0 g.) in a few cc. CCl_4 treated with about 8 cc. 5% CCl_4-Br in small portions during 0.5 hr. and evaporated, the residual yellow oily paste dissolved in 10 cc. Ac_2O, the solution treated with 0.5 g. powdered KOAc, refluxed 3 hrs., treated with iced H_2O, and filtered, the residual creamy paste refluxed 0.5 hr. with 15 cc. 8% alc. KOH, the mixture cooled, poured onto 50 g. ice containing a slight excess of dilute H_2SO_4, and extracted with Et_2O, the extract evaporated, and the residual pale yellow waxy solid triturated during several days at room temperature with a few cc. petr. ether gave 0.04 g. compound A, m. 88.5-9.5°; the filtrate from the isolation of compound A cooled in ice gave 0.30 g. impure compound B, m. 56-61.5°; the crude compound B treated with three 10-cc. portions ligroine at room temperature, the combined exts. concentrated to 10 cc., cooled to 15°, and centrifuged, and the

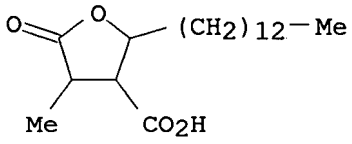
precipitate washed with a little cold ligroine and recrystd. from ligroine at 10° yielded 10 mg. pure cis-2,3-epoxyhexadecanoic acid, flakes, m. 70.0-70.9°. $(CF_3CO)_2O$ (21.2 cc.), 3.5 cc. 90% H_2O_2, and 25 cc. CH_2Cl_2 added with cooling dropwise during 40 min. to 10.6 g. IX, 56.5 g. Na_2HPO_4, and 70 cc. dry CH_2Cl_2, refluxed 0.5 hr., and stirred with 100 cc. H_2O, the aqueous layer washed with 70 cc. CH_2Cl_2, and the combined organic layer and extract washed, dried, and worked up yielded Me tridecylglycidate (X) in 3 fractions: (1) b0.4 140-6°, 3.73g.; (2) b0.4 148-50°, 2.62 g.; (3) b0.4 150-2°, 3.73 g. X (0.2902 g.), 10 cc. dioxane, and 0.5 cc. 10% aqueous NaOH refluxed 1.5 hrs. under N, cooled, poured into iced H_2O containing 5 cc. 5% HCl, and extracted with Et_2O, the extract worked up, and the residual oil diluted with 8 cc. petr. ether, cooled, and filtered yielded 0.122 g. trans-tridecylglycidic acid, platelets, m. 86-7°. Na (0.485 g.) in 8 cc. absolute MeOH treated with 2.79 g. $CH_2(CO_2Me)_2$, the mixture treated during 10 min. with stirring with 6.00 g. X in 10 cc. absolute MeOH, refluxed 4 hrs., cooled, poured into 150 cc. ice and H_2O, acidified with 5% HCl, extracted with $CHCl_3$, and the extract worked up gave 7.85 g. crude, pale yellow, oily product which chromatographed on silicic acid gave pure α,β- dicarbomethoxy-γ-tridecyl-γ-butyrolactone (XI), white wax. XI (2.1 g.) in 40 cc. MeOH treated with 5 cc. H_2O containing 1.84 g. KOH, refluxed 3 hrs., kept overnight at room temperature, decanted, the oily residue dissolved in 50 cc. H_2O, the solution acidified with 5% HCl to Congo red and filtered, and the residue dried (1.182 g.) and recrystd. from 20 cc. hot MeOH yielded 0.721 g. mono-K salt (XlI) of α,β-dicarboxy-γ-tridecylbutyrolactone (XIII), powder, m. 124° (decomposition); the mother liquor poured into 100 cc. H_2O, acidified with 5% HCl, extracted with Et_2O, and the extract worked up gave 0.494 g. white material. XII (0.0394 g.) refluxed 0.5 hr. with 0.5 cc. 5% H_2SO_4, cooled, extracted with Et_2O, and the extract worked up gave 0.0265 g. mixed diastereoisomers of V, m. 87.5-94.5°. XII (0.050 g.) in 5 cc. MeOH acidified with 5% HCl, diluted with H_2O, extracted with Et_2O, and the extract dried and evaporated under N at room temperature gave 0.036 g. XIII. XII (0.372 g.) treated with 0.207 g. Et_2NH and 0.126 g. 30% aqueous CH_2O, diluted with 2 cc. MeOH, heated 1 min. on the steam bath, kept 1 day at room temperature, treated again with 0.126 g. 30% aqueous CH_2O, allowed to stand 1 day, diluted with a few cc. MeOH, evaporated, the residue evaporated twice with $CHCl_3$, the resulting solid kept overnight in 5 cc. $CHCl_3$ and filtered, and the residue (0.114 g.) dissolved in glacial AcOH, treated with a few drops H_2O, cooled to 15°, and filtered gave 0.061 g. dl-protolichesterinic acid (XIV), m. 92.5-4.5° the filtrate from the crude XIV K salt evaporated, the residual semisolid dissolved in 2 cc. dry C_6H_6, the solution kept 3 days at room temperature with 5 cc. MeI, filtered, evaporated at about 40° under N, the residual crude oil (0.338 g.) dissolved in 4 cc. MeOH, the solution treated with 5.5 cc. 5% aqueous $NaHCO_3$, allowed to stand 3 days, diluted with H_2O, extracted with Et_2O, the aqueous solution acidified with 5% HCl and extracted with Et_2O, and the extract worked up yielded 0.0513 g. (crude) XIV, m. 87.5-97.5°. Crude XIV (74 mg.) chromatographed on 5 g. silicic acid gave 29% purified dl-lichesterinic acid (XV), m. 114-15°, 42% XIV, m. 100.5-101.5°, and 11.8% less pure XIV, m. 98.5-100°. XIV (30 mg.) and 5 cc. Ac_2O heated 1 hr. on the steam bath, cooled, diluted with H_2O, and filtered yielded 21 mg. XV, m. 113-15° (AcOH). XIV (20 mg.) in 10 cc. glacial AcOH hydrogenated over 50 mg. 10% Pd-C, filtered, diluted with H_2O, the precipitate recrystd. from

AcOH, and the product extracted with boiling ligroine and recrystd. from AcOH yielded 9 mg. dihydro derivative of XV, m. 114-16°. XII (0.3835 g.), 3 cc. MeOH, 0.079 g. Me2NH.HCl, 0.0873 g. Me2NH, and 0.097 g. 30% aqueous CH2O kept 2 days at room temperature, filtered, treated with a few cc. MeOH, evaporated in vacuo on the steam bath, this procedure repeated twice with the addition and removal of CHCl3, the residual waxy solid treated with 3 cc. dry C6H6 and 5 cc. MeI, the mixture kept 3 days at room temperature, filtered, and the residue (0.653 g.) recrystd. from glacial AcOH yielded 0.340 g. methiodide (XVI), platelets, m. 165° (decomposition); the filtrate evaporated under N, the residual yellow oil (0.126 g.) dissolved in 2 cc. MeOH, the solution treated 3 days at room temperature with 2.1 cc. 5% aqueous NaHCO3 and extracted with Et2O, the aqueous phase acidified with 5% HCl and extracted with Et2O, the extract dried and evaporated, and the residue (0.038 g.) extracted with ligroine and recrystd. from aqueous AcOH gave 0.010 g. V, m. 98-100°. MeOH (5 cc.) and 2.8 cc. 5% aqueous NaHCO3 added to 0.211 g. XVI, kept 3 days at room temperature, diluted with H2O, washed with CHCl3, acidified, extracted with CHCl3, and the extract worked up yielded 0.029 g. XIII, m. 92-5° (AcOH).

IT 102180-12-1, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
(isomers)

RN 102180-12-1 CAPLUS

CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)



L5 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1957:51796 CAPLUS

DOCUMENT NUMBER: 51:51796

ORIGINAL REFERENCE NO.: 51:9566a-c

TITLE: Action of acetyl hydroperoxide on alkylfuryl alcohols

AUTHOR(S): Azanovskaya, M. M.; Pansevich-Kolyada, V. I.

SOURCE: Doklady Akademii Nauk SSSR (1956), 111, 1245-8
CODEN: DANKAS; ISSN: 0002-3264

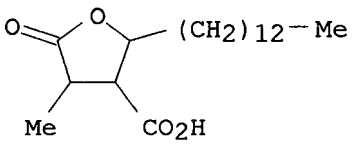
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

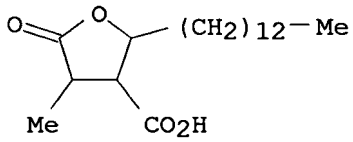
AB Alkylfurylcarbinols were treated with 90-5% AcO2H in Et2O at 20-5° with 1:1 and 1:2 molar proportions of the reactants. With 1:1 mole ratio there were formed 2,3-epoxy-2-furylalkylcarbinols (alkyl group shown): Et, 48%, m. 69.5-71°; Pr, 62.7%, m. 57.5-9.5°; Bu, 72.6%, m. 82-3°; iso-Am, 30%, m. 60-1.5°. Treatment of the Bu compound with ZnCl2 or prolonged storage resulted in decomposition yielding BuCHO. When 2 moles of AcO2H is used for the oxidation only the Bu compound gave a trace of the above described monoepoxy compound The main bulk of the material from such reactions consisted of mixts. of aldehydes and acids. Thus the Bu compds. gave BuCHO, HCO2H, AcOH, and unidentified acids. The Et compound gave EtCHO, HCO2H, and AcOH, as well as unidentified acids. When the reaction was stopped before completion, appreciable amts. of monoepoxy compds. could be isolated.

IT 102180-12-1
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 102180-12-1 CAPLUS
CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)

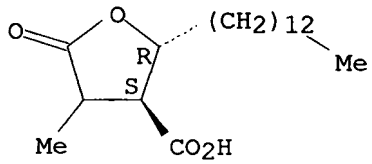


L5 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:51795 CAPLUS
DOCUMENT NUMBER: 51:51795
ORIGINAL REFERENCE NO.: 51:9565i,9566a
TITLE: Synthesis of protolichesterinic acid, dihydroprotolichesterinic acid, and lichesterinic acid methyl ester
AUTHOR(S): Bach, Shirley Rosenberg
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: (1957) 99 pp.;microfilm, $2.00; paper enlargement, $9.90 Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 20222
From: Dissertation Abstr. 17, 501
DOCUMENT TYPE: Dissertation
LANGUAGE: Unavailable
AB Unavailable
IT 102180-12-1P, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone 897946-24-6P, Protolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)
RN 102180-12-1 CAPLUS
CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)



RN 897946-24-6 CAPLUS
CN Protolichesterinic acid, dihydro- (6CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:34628 CAPLUS
DOCUMENT NUMBER: 51:34628
ORIGINAL REFERENCE NO.: 51:6517b-c

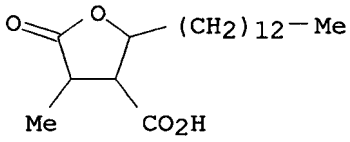
TITLE: Synthesis of (±)-protolichesterinic acid
AUTHOR(S): Van Tamelen, E. E.; Bach, S. R.
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Chemistry & Industry (London, United Kingdom) (1956) 1308
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 50, 6322a). A stereoselective synthesis of (±)-protolichesterinic acid (I) was carried out. Me 2-hexadecenoate with CF3CO3H yielded Me 2,3-epoxyhexadecanoate, b0.4 148-52°. Ring opening with di-Me malonate anion yielded, after spontaneous cyclization of the intermediate γ-hydroxy ester, α,β-dicarbomethoxy-γ-n-tridecyl-γ-butyrolactone. This on hydrolysis with hot MeOH-KOH was converted to the mono-K salt of the diacid, m. 124°, which with HCHO and Et2NH yielded I, m. 100.5-1.5°. Identification was confirmed by 3 separate tests.

IT 102180-12-1P, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)

RN 102180-12-1 CAPLUS

CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)



L5 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:31889 CAPLUS
DOCUMENT NUMBER: 50:31889
ORIGINAL REFERENCE NO.: 50:6322a-i
TITLE: Synthesis of dl-lichesterinic acid methyl ester
AUTHOR(S): Van Tameslen, Eugene E.; Osborne, Clyde E., Jr.; Bach, Shirley Rosenberg
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Journal of the American Chemical Society (1955), 77, 4625-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

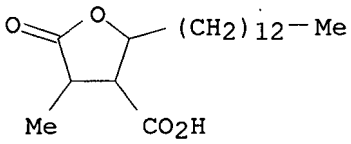
AB The Me ester (I) of dl-lichesterinic acid O.CO.CMe:C(CO2H).CH(CH2)12Me (II) has been synthesized by the SO2Cl2 dehydrogenation of Me ester (III) of dl-dihydroprotolichesterinic acid (IV), which was prepared by the NaBH4 reduction of C13H27COCH(CO2Me)CHMeCO2Me (V). Various transformations encountered in the catalytic reduction of II and protolichesterinic acid (VI) are presented, and the possible biogenetic origins of these substances are discussed. C13H27COCH2CO2Me (VII), m. 38-9°, was prepared in 40% yield by the method of Stallberg-Stenhagen (C.A. 41, 4105d), filtering the crude product by suction with a rubber dam and recrystg. at 0° from petr. ether. VII (5.0 g.), 2.9 g. NaI, and 3.18 g. MeCHBrCO2Et added to 0.41 g. Na in 10 cc. absolute MeOH, the mixture heated a few min. on the steam bath, held 4-7 days at room temperature, poured into H2O, acidified with NaHSO4, and filtered, and the waxy filter residue recrystd. from 30 cc. ligroine (b. 60-8°) gave 4.35 g. C13H27 COCH(CO2Me)CHMeCO2Me (VIII), colorless prisms, m. 49-50°. VIII (5

g.) in 50 cc. absolute MeOH held 3 days at room temperature with 3.9 cc. 1.0M NaBH4 in MeOH, the mixture treated with an addnl. 5.5 cc. NaBH4 solution, allowed to stand 3 hrs., and poured into H2O, the mixture acidified with NaHSO4, the precipitated oil extracted into Et2O, the extract dried and evaporated, the oily residue refluxed 19 hrs. with 3.5 g. KOH in 55 cc. 90% MeOH, the precipitate filtered, dissolved in H2O, and acidified with 5% HCl, the crude precipitate extracted with petr. ether, and the insol. residue recrystd. from glacial AcOH yielded 1.70 g. IV, m. 114-15°; the filtrate of the hydrolysis mixture poured into a large excess H2O and acidified with NaHSO4, the crystalline precipitate dried and extracted with boiling ligroine (b. 60-8°) to remove some II, m. 84.5-5.0°, and the residue recrystd. from glacial AcOH yielded 9% dl-isodihydroprotolichesterinic acid (IX), m. 135-6°. IV treated with CH2N2 gave III, m. 62.0-2.5° (from MeOH). Similarly was prepared the Me ester of IX, m. 67.0-7.15°. d-VI hydrogenated in glacial AcOH at room temperature over 10% PdC, the mixture diluted with H2O, and the precipitate recrystd. from glacial AcOH yielded 60% d-IV, m. 103.5-4.5°; Me ester, m. 54.5-5.5°. VI (1.8 g.) hydrogenated in the same manner gave dl-IV, m. 109-16°. C13H27CH:CHCO2H (8.8 g.) in 500 cc. H2O containing 18.5 g. KOH cooled to 0° with stirring, the resulting suspension warmed to room temperature, treated with stirring during 4 hrs. with 2.50 g. Cl gas, and acidified with an equivalent amount H2SO4, the white solid precipitate dissolved in Et2O, the solution dried and concentrated, the residual pale yellow oil dissolved in 90 cc. ligroine, the solution cooled several days at 0-5°, and the crystalline deposit (2.3 g.) recrystd. from ligroine gave 1.7 g. chlorohydroxydecanoic acid, m. 75.7-6.2°; Et ester, m. 50.8-1.5°. III (200 mg.), 160 mg. SO2Cl2, and 10 mg. Bz2O2 in 0.5 cc. CCl4 refluxed 18 hrs., the solvent removed in vacuo, the residue treated with H2O and 20 cc. Et2O, the Et2O layer dried and evaporated, the residue dissolved in 1 cc. EtOH, the solution filtered, and chilled, and the solid deposit dried and recrystd. from MeOH yielded 7-17% I, m. 49-50°. II (5 mg.) from equal parts of the optical antipodes treated with CH2N2 in Et2O yielded I, m. 51-2°. IV heated with Br in polyphosphoric acid at 120-40° and the resulting product treated with collidine gave an unseparable mixture of products. IV treated with N-bromosuccinimide and Bz2O2 gave crude material containing about 7% II. dl-I (9.6 mg.) in 2 cc. MeOH treated with 1 cc. 2.66 + 10-2M aqueous NaOH, the solution held 5 days at room temperature, acidified with NaHSO4, and filtered, the filter residue dissolved in ligroine, the solution filtered and evaporated, and the residue recrystd. gave dl-II, m. 83-4°. d-II (540 mg.) in 200 cc. glacial AcOH hydrogenated over 200 mg. PtO2, the mixture filtered, the filtrate diluted with H2O, and the precipitate extracted with boiling ligroine and recrystd. 3 times from glacial AcOH yielded 250 mg. C13H27CH(CO2H)CHMeCO2H (X), m. 135.5-6.5°. X (82 mg.) heated 1 hr. at 100° in a sealed tube with 0.4 cc. AcCl, the excess AcCl evaporated, and the residue recrystd. from ligroine, at -78° gave 57% anhydride of X, m. 34°.

IT 102180-12-1P, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)

RN 102180-12-1 CAPLUS

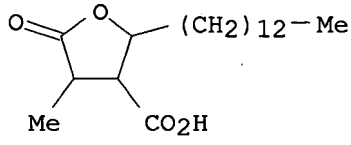
CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)



L5 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1951:39033 CAPLUS
DOCUMENT NUMBER: 45:39033
ORIGINAL REFERENCE NO.: 45:6691h-i,6692a-b
TITLE: Antibacterial effects of lichen substances. I. Comparative studies of antibacterial effects of various types of lichen substances
AUTHOR(S): Shibata, Shoji; Miura, Yoshiaki; Sugimura, Hisako; Toyoizumi, Yuri
CORPORATE SOURCE: Univ. Tokyo
SOURCE: Yakugaku Zasshi (1948), 68, 300-3
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

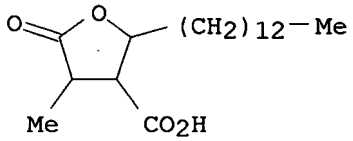
AB cf. preceding abstract The relation between the chemical structure of usnic acid and its antibacterial effects described in previous papers was discussed. Comparatively powerful antibacterial activities against gram-pos. bacteria were found in lichesterinic acid and its derivs. and in depsides from orcinols having large alkyl radicals. No antibacterial activities were found in fatty acids of the caperatic acid type, depsides of the β-orcinol series, depsidones, and endocrocin related to anthraquinone. None showed any activity against gram-neg. bacteria. The highest dilns. inhibiting growth of M. tuberculosis (avian type) and Staph. aureus, resp., were: protolichesterinic acid -, 1:80,000; l-lichesterinic acid 1:40,000, 1:160,000; l-dihydroprotolichesterinic acid 1:80,000, 1:80,000; caperatic acid -, 1:5,000; rangiformic acid -, < 1:5,000; zeorin -, < 1:5,000; lecanoric acid -, < 1:5,000; divaricatic acid 1:10,000, 1:80,000; sphaerophorin -, 1:80,000; anziaic acid -, 1:80,000; perlatolinic acid 1:40,000, 1:80,000; olivetoric acid 1:10,000, 1:20,000; sekikaic acid 1:10,000, 1:80,000; ramalinolic acid -, 1:20,000; boninic acid -, 1:10,000; atranorin -, < 1:5,000; thamnolic acid -, < 1:5,000; lobaric acid -, 1:20,000; salazinic acid -, 1:5,000; psoromic acid -, 1:5,000; fumarprotocetraric acid -, < 1:5,000; pannarin -, < 1:5,000; endocrocin -, <1:5,000.

IT 102180-12-1, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
(antibacterial effects of)
RN 102180-12-1 CAPLUS
CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)



L5 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1949:6300 CAPLUS
DOCUMENT NUMBER: 43:6300
ORIGINAL REFERENCE NO.: 43:1322b-f
TITLE: Lactone aliphatic acids as antibacterial agents

AUTHOR(S): Cavallito, Chester J.; Fruehauf, Dorothy M.; Bailey, John H.
SOURCE: Journal of the American Chemical Society (1948), 70, 3724-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB A study has been made of the relationship between lactone structure and antibiotic activity. The Na salt of α-carbethoxybutyrolactone (18 g.) in 250 cc. absolute EtOH and 0.1 mol. of the alkyl bromide were refluxed 4 hrs., the reaction mixture poured into 500 cc. H2O, extracted with three 150-cc. portions of CHCl3, and the residue saponified with 8.4 g. KOH in 150 cc. EtOH; the yields of the substituted α-carboxybutyrolactones, H2C.CH2.CR(CO2H).CO.O, were from 20 to 45% (R is given): C10H21 m. 75-7° (m.ps. corrected), η (in 0.1 M K phosphate buffer at pH 7; acid concentration 3 + 10-5 millimol./cc.) 70.3; C12H25 m. 78-9°, ε 68.1; C13H27 m. 69-70°, η 43.3; C14H29 m. 82-3°, η 35.0 (γ-Me derivative m. 64-7°, η 33.2); C16H33 m. 80-2°, η 41.4 (γ-Me derivative m. 60-3°, η 37.6). l-Protolichesterinic acid (I) (1.5 g.) and 1.5 g. l-cysteine-HCl in dilute NaHCO3 (pH 7), kept 20 hrs. at 25° and the solution strongly acidified with HCl, give 1 g. of the l-cysteine derivative (II) of I, m. 185-8° (decomposition); the addition appears to be through the SH group. Data are given for the min. bacteriostatic concentration for Streptococcus hemolyticus C203, Staphylococcus aureus 209, Clostridium welchii, Bacillus typhi, and B. tuberculosis ranae and H37Rv for the above lactones, I, II, l-lichesterinic acid, l-dihydroprotolichesterinic acid, and chaulmoogric acid. The antibacterial activity of I is related to its effect on η and not to any significant extent on the unsatd. system. II is much less inhibitory to bacteria than is I. Of the lactones, the C14 chain was optimum in contributing to the antibacterial activity and the γ-Me derivative has about the same activity. The lactone aliphatic acids are more compatible with complex media than are the aliphatic monocarboxylic and malonic acids and are more soluble at neutrality.
IT 102180-12-1, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone of l-
(bacteriostatic action of)
RN 102180-12-1 CAPLUS
CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)



L5 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1939:59734 CAPLUS
DOCUMENT NUMBER: 33:59734
ORIGINAL REFERENCE NO.: 33:8593d-f
TITLE: Constituents of Nephromopsis stracheyi f. ectocarpisma Hue. II. Constitution of nephromopsinic acid
AUTHOR(S): Asano, Mituzo; Yasusumi, T.
SOURCE: Yakugaku Zasshi (1939), 59, 377-83
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

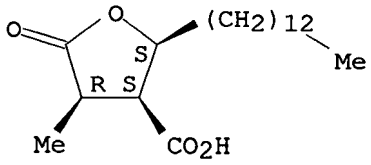
AB cf. C. A. 29, 5072.6. Nephromopsinic acid (I) (2.5 g.) when boiled for 1.5 hrs. with 40 cc. 5% alc. KOH, treated with 6.9 g. $AgNO_3$ in alc. and heated for 2 hrs. at 50° with 15 g. MeI gave nephromopsinic methyl ester (II), m. 59-60°. Hydrolysis of II gave dihydro-l-protolichesterinic acid, $C_{19}H_{34}O_4$, m. 103-5°. Et pelargonoylacetate (6 g.), NaOEt and 5 g. $MeCHBrCO_2Et$ when heated in the sealed tube at 120° for 5 hrs. gave Et α-methyl-α'-pelargonoylsuccinate (III), b3 158-62°. Reduction of 20 g. III with Na-Hg gave 1 g. α-methyl-γ-octylpelargonic acid, $C_{14}H_{24}O_4$, m. 112-14°; hydrolysis of the Et ester gave α-methyl-α'-nonylidenesuccinic acid, $C_{14}H_{24}O_4$, m. 132-4°. Et myristinoylacetate (7 g.), NaOEt and 4.3 g. $MeCHBrCO_2Et$ when heated in the sealed tube at 120-30° for 4 hrs. gave Et methylmyristionylsuccinate (IV). Reduction of 34 g. IV with Na-Hg gave a small amount of α-methyl-γ-tridecylpelargonic acid, $C_{19}H_{34}O_4$, m. 134-6°.

IT 493-45-8, Nephromopsinic acid
(and derivs.)

RN 493-45-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1939:59733 CAPLUS

DOCUMENT NUMBER: 33:59733

ORIGINAL REFERENCE NO.: 33:8593b-d

TITLE: Preparation of acetyl-5-fluorosalicylic acid

AUTHOR(S): Suter, C. M.; Weston, Arthur W.

SOURCE: Journal of the American Chemical Society (1939), 61, 2317-18
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 33:59733

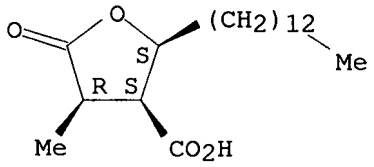
AB Carbonation of the Mg derivative of 2-bromo-4-fluorophenetole gives 64.5% of 2-ethoxy-5-fluorobenzoic acid, m. 65.5-6.5°; refluxing with HI (d. 1.7) for 10 hrs. gives 87% of 5-fluorosalicylic acid (I), m. 178.5-9.5°; $FeCl_3$ gives a purple-violet color; the Me ester has the "oil of wintergreen" odor; Ac derivative (II), m. 130-1°, 56% yield. I is approx. twice as toxic as the F-free acid and II is about 50% more toxic than aspirin. 5-Chlorosalicylic acid has the same germicidal action as the parent acid.

IT 493-45-8, Nephromopsinic acid
(and derivs.)

RN 493-45-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

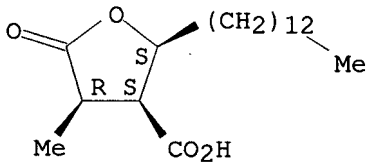
Absolute stereochemistry.



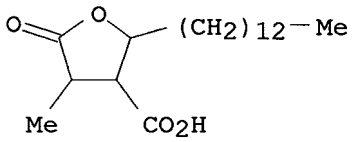
L5 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1939:14245 CAPLUS
DOCUMENT NUMBER: 33:14245
ORIGINAL REFERENCE NO.: 33:2125a-f
TITLE: Constitution of nephromopsinic acid. II
AUTHOR(S): Asano, Mitizo; Azumi, Tiaki
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1939), 72B, 35-9
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 29, 5072.6. When nephromopsinic acid, C19H34O4 (I), which is probably a diastereomer of dihydroprotolichesterinic acid, RC4H.C3H(CO2H).C2HMe.C1O.O (II, R = C13H27), is heated with 2 equivs. of alc. KOH so that the lactone ring is opened and is then treated with AgNO3 it gives a gray-black Ag salt which with MeI yields the Me ester, m. 59-60°, of I, identical with that obtained with CH2N2. On the other hand, saponification of this ester with alc. KOH does not regenerate the original I but l-II, m. 103-5°. As II is formed by hydrogenation of protolichesterinic acid, it must be assumed that the 2-C atom of II is racemized. It follows that alkaline saponification of I opens the lactone ring, to be sure, but does not racemize the 2-C atom; when, however, its ester is saponified, the 2-C atom is first enolized and on acidification II is formed. α-Methyl-γ-alkylparaconic acids (II) were synthesized according to the scheme RCOCH2CO2Et + MeCHBrCO2Et (III) → RCOCH(CO2Et)CHMeCO2Et (+ Na-Hg) → II. From 6 g. Et pelargonoylacetate (IV), b16 149-51°, b2 115°, with III and Na in alc. at 120° was obtained 8 g. di-Et α-methyl-α'-pelargonoylsuccinate (V), b3 158-62°, which gives a faint brown color with alc. FeCl3. The residue from the distillation of IV solidified on long standing and yielded from AcOH tablets of 6-octyl-3-pelargonoylpyronone, m. 70-1°, insol. in alkali and giving no color with FeCl3. V (20 g.) in alc. and water treated in the course of 3 days with Na-Hg with occasional addns. of AcOH to tone down the alkalinity gave about 8 g. acid products which on esterification yielded 1 g. α-methyl-γ-octylparaconic acid (VI), m. 112-14°, and a mixture of esters separated into 4 g. b2 130-60° (VII) and 2 g. b2 164-70° (VIII). Saponification of VII yielded α-methyl-γ-ketolauric acid, m. 62-3° (semicarbazone, m. 125-6.5°), and VIII gave VI. Heated with Na in alc. at 90-100° and then saponified with 5% KOH VIII yielded α-methyl-α'-nonylidenesuccinic acid, m. 132-4°, which immediately decolorized KMnO4. Et myristoylacetate (IX), b3 165-70°; in its distillation there remained a considerable residue of 6-tridecyl-3-myristoylpyronone, m. 85.5-7°, which with HI (d. 1.7) at 160-70° yielded ditridecylpyronone, m. 65-6°. α'-Myristoyl homolog of V (34 g. from 28 g. IX), brownish oil, gave with Na-Hg lichesterylic acid, m. 80-3°, and a little (0.1 g.) of the γ-tridecyl homolog of VI, m. 143-6°.
IT 493-45-8, Nephromopsinic acid
(and derivs.)

RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

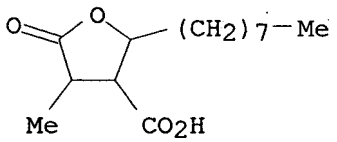
Absolute stereochemistry.



IT 102180-12-1P, Paraconic acid, 4-methyl-2-tridecyl-
854909-07-2P, Paraconic acid, 4-methyl-2-octyl-
RL: PREP (Preparation)
(preparation of)
RN 102180-12-1 CAPLUS
CN Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone (6CI) (CA INDEX NAME)



RN 854909-07-2 CAPLUS
CN Paraconic acid, 4-methyl-2-octyl- (4CI) (CA INDEX NAME)



L5 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1937:21713 CAPLUS
DOCUMENT NUMBER: 31:21713
ORIGINAL REFERENCE NO.: 31:3028h-i,3029a-i
TITLE: Lichen substances. LXXVII. The lichen aliphatic acids from Nephromopsis endocrocea
AUTHOR(S): Asahina, Yasuhiko; Yanagita, Masaiti; Sakurai, Y.
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1937), 70B, 227-35
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB It had been shown (C. A. 29, 7308.5) that Nephromopsis endocrocea Y. Asahina yields, in addition to the yellow pigment endocrocin, a colorless aliphatic acid (I) and a neutral substance (II). I, which was apparently a homogeneous lactonic acid, m. 93-5°, [α]D20 25.46°, proved to be really a mix. of 2 acids, for with KMnO4 it gave lauric acid and a saturated monobasic lactonic acid C17H30O4, designated nephrosteranic acid (III), and on ozonolysis yielded a considerable amount of HCHO,

indicating the presence of a vinyl group (Clemo and MacDonald, C. A. 29, 7939.2). If I is heated with Ac2O, it gives an acid (IV), m. 112°, [α]D24 33.75° (CHCl3), stable toward cold KMnO4 but partly oxidized to lauric acid when heated, leaving III. With boiling alkali IV partially changes into a ketonic acid, nephrosterylic acid, C16H30O3 (V), whose oily oxime gives on Beckmann rearrangement an amide which can be cleaved to undecylamine, m. 20° (Bz derivative, m. 57°), and pyrotartaric acid, m. 112°. On dry distillation IV gives, along with III, an unsatd. lactone, C16H28O2 (VI), which is hydrolyzed by alkali to V; it must therefore be the enol lactone of V and is called nephrosterylolactone. These facts show that III is an original component of I which remains unchanged in all the above reactions. The other (unsatd.) component, which is designated nephrosterinic acid (VII), is reminiscent of protolichesterinic acid (C. A. 26, 5067). To sep. III and VII, I was treated with semicarbazide, which gave, together with III, a semicarbazino compound, C18H33O5N3 (VIII); the free VII could not be regenerated from VIII, but on the assumption that the semicarbazide adds at the vinyl double bond, VII would have the composition C17H28O4. VII was also obtained as a Hg(OH) Cl compound (IX) by treating I with Hg(OAc)2 and then with NaCl; demercurization of IX yielded no well defined product, however. A sharp separation of III and VII was effected by chromatography on Al3O3, the unsatd. VII being retained in the upper part of the Al2O3 while III accumulated in the lower part. On catalytic hydrogenation, the mixture I was completely converted into III; III is therefore a dihydro derivative of VII. VII is accordingly assigned the structure shown in the accompanying formula. By rearrangement it changes into isonephrosterinic acid (X) which on distillation loses CO2 and gives VI. On saponification with alkali,

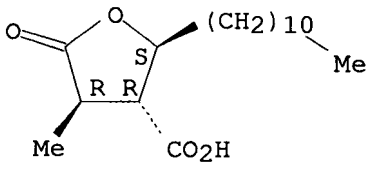
both X and VI yield V, C11H23COCH2CHMeCO2H, whose structure was established by synthesis as well as by the Hofmann rearrangement of its oxime (see above). II is very similar to, perhaps identical with caperin (J. prakt. Chemical 58, 409(1898)); it gives sterol-like color reactions, a property which has not been reported for caperin. III (0.3 g. from 1 g. I in 10% KOH treated with saturated KMnO4 to a permanent violet color), m. 95°, is recovered unchanged when boiled 3 hrs. in 10% KOH and acidified. V, m. 74°, soluble without color in Na2CO3; semicarbazone, m. 117°. VI (2.5 g. from 5 g. IV heated at 200-10° under 15 mm. until the evolution of CO2 ceases and then distilled at 210-30°), b3 185-9°, decolorizes KMnO4. VIII (0.4 g. from 1 g. I), sinters around 150°, decomposes 183-4°, is quite stable to KMnO4 in acetone. IX, m. 95°, very stable to HCl, gives in alc. AcOH HgS with H2S but the filtrate yields only amorphous products. VII, m. 96°, [α]D10 10.81° (CHCl3), instantly decolorizes KMnO4 in acetone. X (0.05 g. from 0.12 g. VII heated 1 hr. in Ac2O at 105°), m. 113°, [α]D11 32.98° (CHCl3), stable to KMnO4 in acetone. Et laurinoylacetate (XI), from Et laurinoylacetoacetate and NH4OH, b10 173-5° gives with PhNHNH2 phenylundecylpyrazolone, sandy powder becoming discolored at 205° and carbonizing around 240°. Heated 4 hrs. in alc. at 120° with Na and MeCHBrCO2Me, XI yields a light yellow oil, b4 180-90°, consisting chiefly of Me Et methyllaurinoylsuccinate, which, heated 8 hrs. with HI (d. 1.7) on the water bath, gives α-methyl-β-laurinoylpropionic acid (= V). II, (C12H20O3)n, m. 248°, [α]D18.5 -100.2° (CHCl3), insol. in KOH, gives no color in alc. with either FeCl3 or bleaching powder, dissolves in hot concentrated H2SO4 with red-brown color changing to dirty green; the CHCl3 solution with a few drops Ac2O and 1 drop concentrated H2SO4 becomes blue-violet, then green.

IT 480-71-7P, Nephrosteranic acid
RL: PREP (Preparation)
(preparation of)

RN 480-71-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L5 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1936:22403 CAPLUS
DOCUMENT NUMBER: 30:22403
ORIGINAL REFERENCE NO.: 30:2945i,2946a-g
TITLE: Lichen substances. LXII. Constituents of Cetraria islandica Ach.
AUTHOR(S): Asahina, Yasuhiko; Yanagita, Masaiti
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1936), 69B, 120-5
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

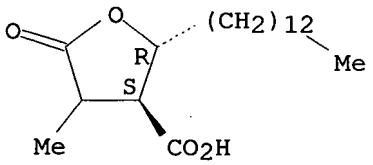
AB cf. C. A. 30, 1041.1. Asano (C. A. 26, 5067) established the structures of protolichesterinic (I) and lichesterinic acid (II), but as he worked not with Cetraria islandica Ach. (III) but with a lichen now considered to be an independent species, C. tenuifolia (Retz.) Howe (IV), the authors undertook a study of the true III, gathered on Mt. Asibetu and morphologically identical in all respects with the European lichen. It contained about 4% of a fatty acid mixture, m. around 90°, [α]D20 -45.62° (CHCl3), from which d-I was readily isolated. The mother liquor then yielded a strongly l-rotatory isomer, l-alloprotolichesterinic acid (V), which gave l-II with hot Ac2O and a pyrazoline derivative with CH2N2, and hence must be structurally identical with I. Heating the fatty acid mixture with Ac2O gave, as expected, dl-II. IV yielded l-I. The fumaroprotocetraric acid, however, which is always found in the European III and in IV, could not be detected in the Japanese III. Theoretically, I has 4 possible different configurations (2 pairs of optical antipodes). There is no reason for assuming a change in the configuration at C atom 4 when I changes into II; l-I would then differ from l-V only in the configuration at C atom 3. Hydrogenation of the I gives, theoretically, 2 dihydro derivs. each, the 8 isomers forming 4 pairs of optical antipodes. Whether the dihydro derivs. obtained from l-I, d-I and l-V are homogeneous or mixts. of 2 diastereomers has not yet been established. d-I, m. 106°, [α]D20 12.07° (CHCl3). V, m. 88°, [α]D23 -56.34° (absolute alc.), [α]D20 -49.53° (CHCl3), instantly decolorizes KMnO4 in acetone. Compound, C21H36O4N2, from V and CH2N2, m. 68-9°, [α]D18 -73.69°, stable toward KMnO4 in acetone. l-II, m. 123°, [α]D20 -25.06° (CHCl3). Dihydro derivative of l-V, m. 92-3°, stable toward KMnO4, [α]D20 -7.41° (CHCl3). l-I, m. 106°, [α]D18 -12.12° (CHCl3); dihydro derivative, m. 106°, [α]D18 -30.96° (CHCl3); pyrazoline derivative, m. 54-5°, [α]D18 -183.1° (CHCl3). Dihydro derivative of d-I, m. 106°, [α]D15 34.60° (CHCl3); pyrazoline derivative, m. 54-5°, [α]D18 190.60°.

IT 249647-94-7P, Protolichesterinic acid, dihydro-
897946-24-6P, Alloprotolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)

RN 249647-94-7 CAPLUS

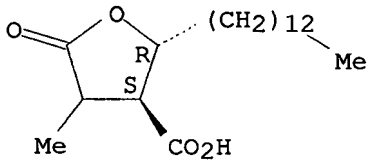
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



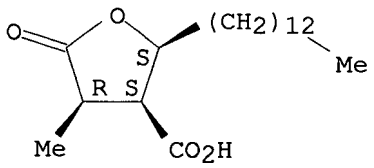
RN 897946-24-6 CAPLUS
CN Protolichesterinic acid, dihydro- (6CI) (CA INDEX NAME)

Absolute stereochemistry.



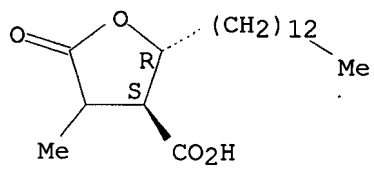
L5 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1935:39202 CAPLUS
DOCUMENT NUMBER: 29:39202
ORIGINAL REFERENCE NO.: 29:5072f-i
TITLE: Constituents of Nephromopsis stracheyi f. ectocarpisma Hue. I
AUTHOR(S): Asano, Michizo; Azumi, Tiaki
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1935), 68B, 995-7
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Extraction of the lichen with ether yields, with 0.03% usninic acid, 1% l-lichesterinic acid and some caperatic acid, 2 new acids, 0.2% of nephromopsinic acid (I), C19H34O4, m. 137°, and an acid C19H30O4 or C19H32O4 (II), m. 106-7°. I is the lactone of a saturated dibasic HO acid (Me ester, m. 60-1°), which with KMnO4 gives a little of a higher fatty acid, and with HI and red P in sealed tubes yields α-methyl-α-tetradecylsuceinanil, m. 63.5-4.5°. I might therefore be α-methyl-λ-tridecylparaconic acid (dihydroprotolichesterinic acid) (III) or tetradecylparaconic acid. Since, however, α-methyl-α'-tetradecylsuccinic acid has been prepared from III (see preceding abstract), I is probably a stereoisomer or diastereomer of III. II immediately decolorizes KMnO4 in AcOH. Its properties agree quite well with those of protolichesterinic acid (IV), but it depresses the m. p. of both d- and l-IV, and with CH2N2 it forms only the Me ester, m. 38-40°, no N-Me derivative
IT 493-45-8P, Nephromopsinic acid
RL: PREP (Preparation)
(preparation of)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1935:39201 CAPLUS
DOCUMENT NUMBER: 29:39201
ORIGINAL REFERENCE NO.: 29:5072d-f
TITLE: Constituents of Iceland moss. V. Reduction of di-hydroprotolichesterinic acid and lichesterinic acid
AUTHOR(S): Asano, Michizo; Azumi, Tiaki
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1935), 68B, 991-4
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Cf. C. A. 26, 5067. λ-Isostearic acid (I), from lichesterinic acid with HI and red P (Boehm, Arch. Pharm. 241, 1 (1903)), m. 48-9°; amide, m. 104-4.5°; anilide, m. 86-6.5°; p-toluide, m. 82-3°. Lichesterylic acid with N2H4.H2O gives 4-methyl-6-tridecylpyridazinone, m. 66°, which with NaOEt at 170-80° smoothly yields I. I was also synthesized by condensing MeCH(CO2Et)2 with NaOEt and pentadecyl iodide to di-Et methylpentadecylmalonate, yellowish oil, b2 197-207°, saponifying the ester to the free acid, m. 95.5-6.5°, decomposing about 175°, and decarboxylating the latter at 170-80°. There can be no doubt, therefore, that I is α-methylheptadecanoic acid. Dihydro-d-protolichesterinic acid, m. 104-6° (Me ester, m. 51.5-2.5°), heated with HI and red P in a sealed tube and then reduced with Zn and AcOH, gives α-methyl-α'-tetradecylsuccinic acid, m. 133-5°.
IT 249647-94-7P, Protolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)
RN 249647-94-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (9CI) (CA INDEX NAME)

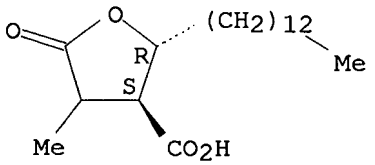
Relative stereochemistry.



L5 ANSWER 53 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1928:37595 CAPLUS
DOCUMENT NUMBER: 22:37595
ORIGINAL REFERENCE NO.: 22:4470g-i,4471a-c
TITLE: Constitution of protolichestearic acid. I
AUTHOR(S): Asahina, Y.; Asano, M.
CORPORATE SOURCE: Tokyo Imp. Univ.
SOURCE: Yakugaku Zasshi (1927), No. 539, 1-17

CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB By Et2O extraction of Cetraria islandica Ach. f. anguslifolia, Kraplh., a subalpine moss in Japan, 1-protolichestearic acid (I), C19H32O4, m. 105°, [α]D27 -12.71°, was isolated in 1.3% yield. It is the optical antipode of the d-acid found in European lichens. I, H2 and Pt black gave dihydroprotolicheslearic acid, C19H34O4, m. 101°. I and H2NCONHNH2 gave the semicarbazone, m. about 140°. These reactions indicate the presence of a double bond in α,β-position to the CO group. Oxidation of I with KMnO4 gave myristic acid, while the oxidation with O3 and subsequent decomposition with H2O gave besides HCO2H and (CO2H)2, α-hydroxypentadecylic acid, C14H28(OH)CO2H. Heating of I with Ac2O resulted in an isometic change and gave 1-lichestearic acid (II), C19H32O4, m. 124°, [α]D25 -32.66°. Heating of II with 10% KOH gave with CO2 evolution, lichesteryl acid (III), C18H34O3, m. 83-4°. III has previously been prepared by Sinnhold (Ann. 55, 144), but the nature of the third O atom remained unexplained. Heating of the oxime of III with H2SO4 resulted in Beckmann rearrangement and gave an acid amide (IV) C18H35(NO3), m. 102°. IV and concentrated HBr in a closed tube gave tridecylamine and methylsuccinic acid. The above reactions show that III has 2 possible structures RCOCH2CHMeCO2H or RCOCHMeCH2CO2H(R = Me(CH2)12-). Heating of II in a vacuum at 20 mm. and 210° gave lichesteryl lactone (V), b. 207°, which on saponification with KOH gave III. V, H2 and Pd-BaSO4 gave the dihydro derivative of V, m. 37-8°, while V, O3 and H2O gave AcOH as a decomposition product. Contrary to the view of Boehm (Arch. Pharm. 241, 1) V is therefore unsatd. The above reactions show that the relation of III to V is like that of levulinic acid to angelic lactone. Hence V has one of the following 4 possible structures: (a) R-CH.CH:CMe.CO.O, (b) R-C:CH.CHMe.CO.O, (c) RCH.CMe:CH.CO.O, (d) RC:C.Me.CH2.CO.O. But the fact that the ozonide of V gave AcOH instead of (CO2H)2 favors the structure (a) for V, while III should have the structure, RCOCH2CH(Me)CO2H. I, therefore, has one of the 2 possible structures, RCH.CH(CO2H).C(:CH2)CO.O or RCH.C(CO2H):CMe.CO.O. Since the ozonide of I gave HCO2H and (CO2H)2 instead of AcOH, the former structure is preferred. From the fact that I did not give III, but II gave III by saponification with an alkali, the following structure is assigned for III.
IT 249647-94-7P, Protolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)
RN 249647-94-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.67	651.88

```
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -24.96     -43.68

FILE 'STNGUIDE' ENTERED AT 09:42:36 ON 27 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Sep 24, 2007 (20070924/UP).

=> d his

     (FILE 'HOME' ENTERED AT 09:23:46 ON 27 SEP 2007)

     FILE 'REGISTRY' ENTERED AT 09:23:58 ON 27 SEP 2007
L1              STRUCTURE UPLOADED
L2            1 S L1
L3           53 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 09:24:48 ON 27 SEP 2007
L4           73 S L3 FULL
L5           53 S L4 AND PY<2002
L6              STRUCTURE UPLOADED

     FILE 'REGISTRY' ENTERED AT 09:29:07 ON 27 SEP 2007
L7              STRUCTURE UPLOADED
L8            5 S L7 FULL

     FILE 'CAPLUS' ENTERED AT 09:29:29 ON 27 SEP 2007
L9            4 S L8 FULL

     FILE 'STNGUIDE' ENTERED AT 09:29:55 ON 27 SEP 2007

     FILE 'CAPLUS' ENTERED AT 09:32:24 ON 27 SEP 2007

     FILE 'STNGUIDE' ENTERED AT 09:32:31 ON 27 SEP 2007

     FILE 'CAPLUS' ENTERED AT 09:40:42 ON 27 SEP 2007

     FILE 'STNGUIDE' ENTERED AT 09:42:36 ON 27 SEP 2007

=> log y
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    0.60     652.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00     -43.68

STN INTERNATIONAL LOGOFF AT 09:48:50 ON 27 SEP 2007
```